Heat and Mass Transfer in Dispersed Two-phase Flows

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Abstract

Industrial and manufacturing processes are an abundant source of rich and complex problems amenable to investigation with mathematical logic and techniques. Once a problem is identified and the right questions are formulated, a range of mathematical modelling methodologies can be leveraged. These methods can be used to simplify the problem to gain valuable insight into the underlying physical mechanisms of the system under consideration. The resulting formulated model can be used to explain observed phenomenon, explore poorly understood behaviour, determine optimal parameters and predict future states of the system. In this thesis, two problems relating to industrial processes are studied.

Consistently extracting the desired level of soluble material from ground coffee with hot water is a key objective in any coffee brewing method. In this study, a coffee extraction model is derived from first principles, using volume averaging techniques, with a view to relating the quality of brewed coffee with the parameters of the underlying processes. Physical mechanisms for the dissolution and transport of coffee are included. The model is parametrised with experimental data for different extraction experiments. The model is non-dimensionalised, to establish the dominant mechanisms during brewing. Numerical and asymptotic solutions are presented.

The hydration process is a key step in the production of soft contact lenses. Hydration primarily involves the removal of leachable chemicals, used as process aids during earlier manufacturing stages, from the contact lens. The leachable materials are removed by washing the lenses with a solvent. In this work, macroscopic models of heat and mass transport in the hydration process are formulated based on experimental data. The heat transport equations are leveraged to estimate the size of heating units required to maintain the specified process temperatures. Chemical transport in the hydration process is modelled with a view to optimising the system parameters.
Declaration

I hereby declare that this thesis is my own work and that it has not been submitted for any other academic award.

The work in this thesis was conducted from September 2013 to August 2016 under the supervision of Dr. William Lee and Prof. Stephen O’Brien in the department of Mathematics and Statistics in the University of Limerick.

Kevin M. Moroney

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To my brother Michael, greatly missed, fondly remembered.
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Mathematics is the fundamental building block underpinning existing knowledge and driving new cutting-edge research and development in the sciences and engineering. The application of mathematics and mathematical logic and reasoning, is an integral part of the journey from the identification and description of an initial problem, right through to the final solution. The translation of a particular problem, or process of interest, into the language of mathematics, is the first and arguably key step in the path towards a solution to a problem or greater understanding of a process. Such a description or model is a representation of a process, usually in the form of a set of equations describing a number of variables of interest. A model is usually founded on observations of a particular phenomenon of interest, which leads to a hypothetical mechanism which can explain the observed behaviour. The establishment of a well-defined model removes any ambiguity from the proposed mechanism and allows the use of well-established and powerful mathematical techniques to analyse, simplify and solve the proposed model. The mathematical solution is then interpreted and translated back into practical information in the situation of interest. If the model is found to reliably reproduce experimental observations, it may be considered validated and used for prediction, within its range of validity. Otherwise efforts may need to be made to improve the model, or it may need to be totally discarded and a new model proposed. This is an iterative procedure and may require a great deal of effort and time. The process of developing the final mathematical model used is
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termed mathematical modelling.

Mathematical modelling finds a natural home in dealing with problems arising in industrial processes. In this context, it is often referred to as industrial mathematics. The applications in industry are broad. Intelligent use of mathematical modelling during the design of industrial equipment and processes can flag any potential problems and oversights, before they become expensive mistakes. The incorporation of mathematical modelling in the design process from an early stage can limit the number and variety of experiments that need to be set up to explore the optimal system parameters in the design space. Modelling can also be used to investigate problems and explore possible solutions on existing processes and equipment. When problems arise in such cases, it becomes important to understand the underlying physical mechanisms of the problematic process which may have been unnecessary previously. This can be done through identification of the appropriate physical models. More recently, mathematical modelling, such as model predictive control (MPC) \[47\], is being increasingly used for on-line process control in industrial manufacturing processes. The application of industrial mathematics offers industrials an opportunity to gain a competitive advantage over their rivals by increasing the performance and efficiency of their systems. The rich and varied problems which arise in industry are equally beneficial to the applied mathematician, who is introduced to new areas and subjects to apply their skills and broaden and develop their knowledge of mathematical techniques.

When dealing with real world problems such as those in industry, it is important to bear in mind that all models are idealisations and will be limited in their applicability. The choice and complexity of a model should be commensurate with the question being asked. Usually it is advantageous to begin with the simplest model which is sophisticated enough to capture the key characteristics of a particular system. The simpler the model, the simpler the analysis. In addition, when the model complexity needs to be increased, the analysis can be informed by that conducted in the simpler case. When formulating a model, it is important that the right question is being addressed. The correct solution to the wrong question may be very elegant, but is unlikely to be useful in the situation of interest. Asking the wrong question initially can lead to the implementation of the wrong models and inhibit or completely block the path to solution. Sometimes, where the aim is to identify the physical mechanism of a particular
1.1 Mathematical modelling of the coffee brewing process

Freshly brewed coffee is an integral part of the daily lives of millions of people across the globe. Coffee is a dilute solution of hot water and soluble material extracted from roasted and ground coffee beans. There are a wide variety of techniques to brew coffee, but all techniques rely on solid-liquid extraction as their central operation. Here, we are particularly interested in an infusion method called drip filter brewing. In this method, ground coffee is placed in a filter and hot water is poured over the coffee bed. The hot water flows down through the process, a bottom-up model needs to be derived from first principles. However in other cases this is unnecessary. For example, often a system only needs to be analysed on a macroscale, rather than modelling each individual component or sub-system. Such a top-down model is phenomenological in nature and so model parameters have to be fitted from available data. Both top-down and bottom-up methodologies will be utilised in this thesis.

In this work, problems from two different industries are considered. The first problem, detailed in part I of the thesis, considers flow and extraction in packed coffee beds. The second problem, considered in part II of the thesis, deals with heat and mass transfer in a sub-system of the manufacturing process for soft contact lenses called the hydration system. On the surface the problems seem unrelated, but in fact they have a common scientific basis. Both problems consist of a solid phase (solid coffee grains or soft polymer lenses) which is dispersed in a liquid phase (hot water or hydrating fluid). The liquid phase flows over the solid phase leaching soluble content. For the coffee bed, the soluble content is the desirable material, which dissolves in the water to produce the coffee beverage. In the case of the contact lens, the soluble content is an unwanted by-product from earlier manufacturing stages. Nevertheless the target in both cases, is the separation of soluble content from an insoluble solid matrix, via solid liquid extraction. This is a common operation in industry with applications varying from the extraction of sugar from sugar beet using water, to the separation of metal from ores using acids. Both problems here fall into the general category of heat and mass transfer in two-phase flows.
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bed under the influence of gravity, soaking into the grains and leaching soluble material. A coffee bed in a conical filter, following extraction, is shown in figure 1.1. Consistently brewing high quality coffee is a significant challenge. The complex chemistry of coffee makes it difficult correlate its properties with taste. Currently, filter coffee machine design is driven by empirical research, which involves trial and error and feedback from expert coffee tasters. This is a time consuming and expensive endeavour and provides little guarantee that the resulting design can robustly produce good coffee. Ideally coffee machine designs would be optimised by computer and adaptable to different coffee grinds and brewing parameters. This would result in significant saving of time and money for companies who manufacture filter coffee machines and better quality coffee for end users. A key obstacle to this ideal, is the lack of mathematical models which can be used to predict the coffee quality of a given design and test its robustness to changes in the brewing parameters. The development of such a model is a challenging undertaking. Ideally, any such model should account for the chemical composition of the coffee used (as determined by its origin and roasting conditions), the microstructure and geometry of the coffee bed and the nature of the flow of hot water (and possibly coffee grains) in the filter. It also needs to be possible to interpret the model output as good or bad tasting coffee.

Chapter 2 is devoted to deriving a general model of coffee extraction from a static, water saturated coffee bed. The model accounts for the doubly porous nature of the coffee bed, which consists of pores between the grains, but also smaller pores within the grains. Multiscale modelling techniques, such as volume averaging, originally developed in the context of groundwater flow, are leveraged to derive the equations describing the extraction and transport of coffee during brewing. The initial model derivation presented here, can be extended to account for unsaturated flow during the initial water infiltration and also to allow transport of solid coffee grains with the flow. Chapter 5 considers the former while the latter extension is not considered here as there is limited data available with which to validate any proposed model. The focus is on parametrising and
validating the general model in the case of two coffee extraction experiments: in a well stirred dilute suspension of coffee grains and in a packed coffee bed. Specialising the general model based on experiments, coffee extraction is divided into two regimes. In the first, a rapid extraction occurs from the surface of the coffee grains, which yields the highest concentrations at any stage of the brewing process. In the second there is a slow extraction at lower concentrations from the interior of the grains. Numerical solutions of the model show that it can quantitatively model extraction in the case of the two experiments discussed above. The work in this chapter is published in the Journal of Chemical Engineering Science [51]. It is also the subject of a conference paper in Progress in Industrial Mathematics at ECMI 2014 [50].

1.1.1 Coffee extraction in a well mixed system

In chapter 3, the general coffee extraction model from chapter 2 is specialised to describe extraction from a dilute suspension of coffee grains. The dominant mechanisms during the extraction are then identified by non-dimensionalising the equations. Approximate solutions are formed, based on the dominant processes during different stages of the extraction. The approximate solutions are compared with numerical solutions of the system and also with experimental data presented in section 2.2.3. The work in this chapter is published in the Journal of Mathematics in Industry [49].

1.1.2 Coffee extraction in a packed coffee bed

In chapter 4 the general coffee extraction model from chapter 2 is specialised to describe extraction from a packed coffee bed. The system of equations is non-dimensionalised to identify the dominant mechanisms during coffee extraction. Approximate solutions can be found based on the dominant mechanism of extraction during different stages of the brewing process. Solutions can be found for both fine and coarse grinds in the two experimental situations outlined in section 2.2.4. Based on these experiments, approximate solutions are developed for coffee extraction from a flow-through cylinder similar to that found in an espresso machine, except the water is at a much lower pressure. In this case, solutions for extraction of fine and course grinds differ due to a difference in the assumed initial coffee concentration in the coffee bed. Solutions are presented for both
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fine and coarse grind parameters. Such solutions can be used to predict the coffee quality (coffee concentration and extraction yield) for a particular brewing configuration with a given set of process parameters. The work in this chapter has been accepted for publication in the SIAM Journal of Applied Mathematics and is currently in press [48].

1.1.3 Infiltration into a dry coffee bed

In chapter 5, the problem of the initial water infiltration into a dry coffee bed, which was neglected in chapters 2–4, is considered. In previous chapters, it had been assumed that the coffee bed was saturated and the bed parameters, following the initial filling stage, were known. The reason for this, is that the water infiltration stage is very complicated to model, with several active processes occurring. For a pressurised flow, the initial contact of water with the dry porous bed leads to significant compaction, changing the bed porosity and resistance to flow. As water enters the bed and infiltrates into the fibrous cellular grain structure, it may induce considerable grain swelling. Coupled with this, coffee grains, particularly if freshly ground, can contain a significant amount of trapped carbon dioxide following roasting. The influence of the competing processes of carbon dioxide evacuation and water infiltration is unclear. A significant amount of work is still to be done in modelling water infiltration at an individual grain scale. With ongoing water penetration into the bed, the counter pressure of the bed builds up, reducing the flow rate, until the bed is saturated.

In this chapter, some simple models of water infiltration into a porous bed are considered including empirical models such as Horton’s equation and Philip’s equation and physical models such as Richards’ equation and the Green-Ampt model. A simple moving boundary infiltration model, similar to the Green-Ampt model, is presented and coupled with coffee extraction equations, in the saturated part of the bed. The model is non-dimensionalised and asymptotic and exact solutions to the infiltration problem are found. The coupled infiltration and extraction model, is solved numerically to estimate the initial concentration profiles in the coffee bed, following infiltration. These profiles are compared with those estimated in earlier chapters.
1.2 Mathematical modelling of a contact lens hydration process

A contact lens is a thin lens which is placed directly on the surface of the eye. In this work, we consider a soft contact lens manufacturing process, which uses a cast-moulding technique. Cast-moulding involves compressing a liquid monomer solution between two moulds, which define the shape of the lens. The liquid solution is cured under UV light and polymerises, forming a soft-solid lens. Some of the constituent chemicals used in the lens formation need to be removed at this stage. This is done by washing the lenses with one or more solvents to leach the unwanted chemicals from the lenses. This process is called the hydration process and the lenses leaving the hydration system are hydrated with water. In chapter 6 the hydration process under consideration in this work is introduced and described in detail. The unwanted component is insoluble in water, so the hydration process is a two-stage extraction. First the lenses are washed with an organic solvent to remove the unwanted component. Following this, the lenses are washed with deionised water to remove the organic solvent. The key questions in the context of heat transport and chemical transport within the system are presented.

1.2.1 Heat transport in the contact lens hydration process

The fluids used in the hydration system must be maintained within a specified tolerance of a set point temperature, in order to ensure an effective and uniform extraction of unwanted leachable content from the lenses. The heating units on the hydration system need to be sufficiently large in order meet the instantaneous energy demands required to maintain the set point temperatures. However oversizing the heaters is also undesirable due to space constraints on the hydration system, as well as increased purchase and running costs. In chapter 7 the problem of choosing the size of the heating units is explored. Heat transport and losses in the system are described by splitting the
1. OVERVIEW

system into energy compartments and modelling the energy transport and losses within and between compartments. By identifying the energy losses at different locations in the system, the energy demand to maintain the set point temperatures during the process can be estimated. A number of models of increasing complexity are proposed. The models are parametrised and fitted with available experiments from a scaled down version of the real production process. Unfortunately idealised control of the heaters is not practical, and in practice the heaters are controlled according to a proportional-integral-derivative (PID) algorithm. The models are adjusted where possible to account for this. Once the models are validated with the available data, the model description and parameters are adjusted to describe the production line process. The output of the models is an estimate of the required size of each of the heating units on the production line hydration system.

1.2.2 Chemical transport in the contact lens hydration process

The primary objective of the hydration section of the contact lens manufacturing process is to leach unwanted chemicals from the contact lenses. In the hydration process considered here, the unwanted chemical is a diluent called 3,7-dimethyl-3-octanol (D3O). This chemical is removed by washing the lenses in number of successive stages with an organic solvent called propylene glycol (PG). Following this, the PG is removed from the lenses by washing them with deionised water (DI), again in a number of successive stages. In chapter 8 the extraction and transport of D3O with PG in the hydration system is modelled using compartment models. Based on experimental data, extraction from a lens is modelled as a diffusive process. The extraction models are fitted with available data from a scaled-down version of the production line process. Once this has been done the models are applied to the production process. The models are used to investigate the influence of various situations and system parameters on the final concentration of D3O in the hydrated lens, with a view to reducing costs. The influence of the flow rate of fresh PG solvent to the system on the extraction and the possibility of recycling PG solvent to reuse in the system are both considered. One of the system’s possible failure modes is a fully or partially blocked solvent dosing nozzle over part of the extraction time. The impact of this is investigated.
In the hydration system the lenses are placed in trays which are stacked one on top of the other. Increasing the number of trays in these stacks means more lenses can be washed. However, experimental data shows that lenses extract less at the bottom positions in the stack than the top. Increasing the stack height may emphasise this. The question of the optimum stack height is considered. Available data on extraction of PG with DI is very variable and so the extraction mechanism cannot be identified. For this reason, no in-depth modelling of this part of the hydration process is attempted.
1. OVERVIEW
Part I

Mathematical modelling of the coffee brewing process
CHAPTER 2

MATHEMATICAL MODELLING OF
THE COFFEE BREWING PROCESS

2.1 Introduction

Coffee is a popular beverage prepared from the beans (seeds) of the coffee plant. The consumption of coffee is on a global scale and has been experiencing a period of strong growth in recent years. In 2010 coffee production reached 8.1 million tonnes worldwide, which represents more than 500 billion cups \[21\]. Typically the preparation of coffee involves three keys stages. First the raw coffee beans are roasted. During roasting, the coffee seeds undergo a number of physical and chemical changes \[21\]. As a result of these changes, the coffee seeds gain their characteristic flavour and aroma. The exact roasting conditions applied have a strong influence on the extraction properties during the subsequent brewing process. The influence of the roasting conditions on the characteristics of the resulting coffee seeds has been the subject of significant research. Some of this work is detailed in refs. \[20, 30\]. Following roasting, the roasted beans are ground down or milled to facilitate a faster extraction during the final brewing stage. The brewing stage involves the leaching of coffee solubles from the roasted and ground coffee grains with hot water. Generally the extracted solution is filtered to remove undissolved solids before consumption. The resulting solution of hot water and coffee solubles is called coffee.
Coffee preparation and consumption habits vary widely and many different local practices can be observed from country to country. Coffee was first consumed in the West in the middle of the seventeenth century [36]. Since then, a wide variety of coffee brewing techniques have been developed. These brewing methods fall into three broad categories: decoction methods, infusion methods and pressure methods. Many of these brewing techniques are described in refs. [54, 55]. In this study we will be particularly interested in an infusion method called drip filter brewing. The preparation of drip filter coffee involves pouring hot water over a bed of coffee grounds in a filter, leaching soluble content. Despite the wide variety of methods used to brew coffee, each method relies on solid-liquid extraction as its central operation. Solid-liquid extraction or leaching is defined as a separation process effected by a solvent, and involving transfer of solutes from a solid to a fluid [2]. Despite its long history and well developed techniques consistently brewing high quality coffee remains a difficult task. Even in its simplest manifestations the brewing of coffee is a complex operation, dependent on a large number of process variables. Some important parameters include the brew ratio (dry coffee mass to water volume used), grind size and distribution, brewing time, water temperature, grain agitation, water quality and uniformity of extraction [54, 57]. According to Clarke [15], “The extraction of roast and ground coffee is, in fact, a highly complex operation, the scientific fundamentals of which are very difficult to unravel”. This is reflected in the absence of a satisfactory, experimentally validated, mathematical system of equations to model the extraction process accurately. Such a description would have obvious benefits in quickly and easily investigating the influence of various parameters on coffee extraction and informing the design of the next generation of coffee brewing equipment. A fundamental goal of this study is to develop such a model which can relate the quality of the final coffee beverage to the parameters of the brewing process. This raises the question of how to define the quality of a brewed coffee beverage.

2.1.1 Defining coffee quality

A fundamental goal for the manufacturers of coffee brewing machines, and end users of their products, is to be able to consistently brew the highest quality coffee possible. This presents a number of challenges. First of all coffee quality is difficult to define and to some degree a matter of taste. In addition to this, even
if the composition of the extracted coffee solution can be identified for different tastes, the coffee machine should be able to change the brewing parameters to move between these ideal compositions. To achieve this goal, both a model relating the final composition of the brewed coffee to the process parameters, and a measure of the quality of the brewed coffee, are required. The complex chemistry of coffee makes it difficult to find correlations between the individual chemical constituents of the extracted coffee solubles and the quality of the final beverage. Coffee is composed of over 1800 different chemical components [54] and the influence of very few of these on taste is known. Despite this, certain correlations have been identified between coffee flavour and extraction yield. Extraction yield is the percentage of the dry coffee grind mass that has extracted as solubles in the final coffee beverage. Extraction yield is the current method used by the coffee industry to quantify extraction. Target ranges of extraction yield and brew strength for filter coffee have been established by speciality coffee associations around the world through organised taste tests. Brew strength is the ratio of the mass of dissolved coffee in the beverage to volume. It is worth noting that some practitioners prefer to measure brew strength on a mass per mass basis, as water density changes with temperature. The ideal extraction yield is generally agreed to be 18–22%. This was originally established by the Coffee Brewing Centre in the United States in the 1960s [41, 57]. More recently the Speciality Coffee Association of Europe (SCAE) produced a report titled “European Extraction Preferences in Brewed Coffee” which confirmed the ideal range. The recommended brew strength varies between regions. The SCAE report an ideal range of 1.2–1.45%, the Speciality Coffee Association of America (SCAA) report an ideal range of 1.15–1.35%, while the Norwegian Coffee Association (NCA) report an ideal range of 1.3–1.55%. The extraction yield and brew strength are related by the brew ratio (mass of dry coffee bed to volume of water used). The brew strength is given by the brew ratio times the extraction yield. More precisely the volume of liquid in the brew ratio should be adjusted for the volume of water retained by the bed. This may be as high as 2 ml per gram of dry coffee. This set of quality standards is usually represented on a chart called the coffee brewing control chart. The chart with SCAE target ranges is shown in figure 2.1.

The chart plots the extraction yield on the horizontal axis and the brew strength on the vertical axis. The regions in the plane are classified according to the quality of coffee produced. Coffee which is below an extraction yield of
18% is classified as underdeveloped. This coffee is under-extracted. As the soluble components of coffee extract at different rates, a low extraction yield tends to favour molecules with a low molecular mass. Such extraction yields favour acidic and sweet components \cite{54}, highlighting sharp, fruity, peanutty and grassy tastes \cite{57}. In contrast, coffee with an extraction yield over 22% is classified as overdeveloped. This coffee has been over-extracted. In this case slower extracting substances with a higher molecular mass begin to dominate extraction. These substances tend to highlight bitter and astringent flavours in the beverage. In between, is the ideal region where compounds extracted highlight mellower tones, riper fruit notes and caramel sweetness \cite{57}, before bitter compounds start to dominate. The strength preferences are similarly classified on the vertical axis.

For the European (SCAE) standards, beverages with concentrations below 1.2% are considered too weak, while beverages with concentrations above 1.45% are considered too strong. The ideal region within specified extraction yield and strength ranges is indicated at the centre of the chart. It is worth noting, that in order for the final coffee beverage to be within the ideal region, the minimum requirement is that a brew ratio between 50 g l\(^{-1}\) and 70 g l\(^{-1}\) is chosen. Following this, it is a matter of selecting the correct combination of coffee grind and brewing parameters to achieve target ranges. Given that the most widely used measure
of coffee quality considers coffee as a single component, it seems logical to model extraction based on a single coffee constituent. Modelling of the coffee concentration (brew strength) and extraction yield of the final beverage for a particular brewing apparatus, with the process parameters as inputs, could be a valuable tool in order to choose the optimal set of parameters to achieve a targeted coffee quality on the coffee brewing control chart. Before considering previous research on coffee extraction, we consider some of the process parameters which influence extraction.

### 2.1.2 Factors influencing coffee extraction

There are a large number of factors which influence the extraction rate and quality during coffee brewing. We will briefly discuss some of them here, mainly in the context of drip filter brewing:

1. Coffee grind size and uniformity

   - **Grind size:** The average size of the coffee grounds influences the extraction rate. Coarser grinds need a longer dwell (extraction) time for ideal extraction compared to finer grinds. In extraction from granular beds, water moves much faster through a coarser grind than a finer grind. In general, to achieve the same extraction level with a coarser grind requires a longer brewing time. Thus particle size dictates brewing time. Conversely for a fixed brewing time and desired extraction level the correct grind size needs to be chosen. So brew time can also dictate grind size.

   - **Grind uniformity:** In order to ensure an even extraction, one would assume that a uniform grain size would be optimal. However, in reality grind size distributions tend to be bimodal, with a significant quantity of very fine particle fragments produced during grinding. As these particles will extract at different rates, the extraction will not be uniform from grain to grain. However in infusion methods, the resulting high specific surface area of the grind helps resist flow and increase the residence time of water in the bed. Thus there is some debate over the importance of having a narrow grind size distribution. Some coffee professionals believe that the uneven extraction may enhance the complexity of the coffee produced [57].
2. CONTACT TIME

Contact time is generally defined as the time between the instant the water first contacts the bed until the flow from the bed reduces to a drip. This includes the initial wetting phase before extraction. Setting the correct contact time for a given grind size is crucial in order to get the ideal extraction yield.

3. TEMPERATURE OF WATER

The extraction rate of coffee, as a dissolution process, depends on the temperature according to the Arrhenius equation [36]. This means coffee extracts faster at higher temperatures. However, setting the temperature too high may produce coffee that is bitter or astringent [57]. For drip filter brewing SCAE recommend a water temperature of 92°C to 96°C in the water entering the bed while ref. [57] recommends a slurry temperature of 91°C to 94°C, adding that temperatures below this may result in sour-tasting coffee.

4. GRAIN AGITATION/WETTABLENESS/Bed depth:

- Mixing and agitation of grains leads to increased extraction as particles separate and are possibly transported around the coffee bed.
- The coffee wettability can be influenced by the roasting conditions. Freshly roasted coffee has large amounts of trapped carbon dioxide gas in the grains’ cellular structure. The initial release of this gas can lead to a delayed wetting. However the mixing of particles caused by the carbon dioxide as it escapes the bed may increase extraction uniformity. The total amount of water absorbed by the particles is also important. This is typically 2 ml per gram of dry coffee, but can be higher or lower depending on the properties of the coffee or water used [1].
- In drip filter brewing, the coffee bed depth should be sufficient to prevent the formation of channels in the bed but shallow enough to allow for grain swelling and ponding. Bed depths of 2.5 cm to 5 cm are recommended.

5. WATER QUALITY

Water should of course taste good, be free of odour and clear. The water chemistry is also important, with specified ranges recommended for total dissolved solids and calcium hardness [1].
6. Optimal brewing method and filtering method: The grain size and other parameters should be chosen with the brewing method in mind and vice versa. The filter paper should be white (not brown) so as not influence the taste of the coffee [1]. In drip filter brewing the water delivery method also has a strong influence on extraction. Water can be either delivered by a single jet to the centre of the bed or by multiple jets of a shower-head over the bed.

2.1.3 Previous coffee research

Given its widespread consumption, coupled with the complexity of the underlying processes, it is not surprising that coffee brewing has been subject to extensive research. In particular the chemistry of coffee brewing has received a great deal of attention, with extensive texts such as [14] and [29] exploring the chemical constituents which make up green and roasted coffee beans. In comparison the physics of coffee brewing has received relatively little attention. Very often, as in other food engineering applications, the importance of the microstructure in mass-transfer is ignored in extraction models and solids are treated as “black boxes” [2]. Some work has been done on modelling extraction in certain brewing systems. Industrial scale coffee extraction to produce instant coffee has been studied with the aim of optimising the design of these systems. Early work [68, 70] looked at models of coffee extraction in large packed columns, called diffusion batteries, with the aim of extracting a highly concentrated solution. In these systems, extraction was performed by forcing hot water through the columns to extract solubles. In order to achieve the maximum possible concentration in the extract, extraction was performed at high temperatures and columns were connected consecutively in a series. Much of this work is summarised in ref. [15].

At a smaller scale some investigation and modelling has been done on domestic and catering brewing systems. Experiments on the operation and efficiency of the stove-top or Moka pot are detailed in ref. [31, 52]. Fasano et al. have developed some very general multiscale models of coffee extraction in different situations, with a particular focus on the espresso coffee machine [23, 24, 25, 26, 27, 28]. A schematic of the espresso process is shown in figure 2.3a. This multiscale approach is reflective of the presence of multiple length scales in the coffee bed due to its doubly porous nature. Large pores exist between the grains, while smaller
2. MATHEMATICAL MODELLING OF THE COFFEE BREWING PROCESS

Figure 2.2: SEM images of roasted Arabica coffee beans from Papua New Guinea at different magnifications: (a) Scale bar reads 20 µm. (b) Scale bar reads 100 µm. Thanks to Rebeckah Burke, University of Rochester for generously agreeing to allow the reproduction of these images. These and further images are available at [58].

Pores exist within the grains. Roasted coffee beans have cells of 20 µm average diameter and a porous structure that is easily apparent in SEM (scanning electron microscope) images [2]. Some sample SEM images of a roasted coffee bean at different magnifications are shown in figure 2.2. Further images can be found in refs. [2, 44, 57]. The influence of some brewing parameters on coffee extraction was investigated by Voilley et al. [72]. A number of different extraction experiments was conducted on a well-mixed system of coffee grounds and water. The response of brew strength to variations in process parameters such as brewing time, granule size, brew ratio and water temperature was considered. A simple model was used to describe the variations of brew strength during the experiments. The model assumed the coffee grains were spherical and suspended in a homogeneous system. Extraction was then modelled as diffusion of a single component from a sphere with a diameter equal to the mean grain diameter. The model was fitted to the data using the diffusion coefficient as a fitting parameter and was found to provide reasonable agreement with the experimental extraction curve. It was noted, however, that the initial extraction proceeded at a faster rate in the experiment compared to the model extraction curve.

There has been very little investigation into the drip filter brewing system. This is surprising as drip filter machines account for about 10 million out of a total of over 18 million coffee machines sold in Europe each year [11]. In this
Figure 2.3: (a) Espresso coffee is made by forcing hot water under high pressure through a compacted bed of finely ground coffee. (b) Drip filter brewing involves pouring hot water over a loose bed of coarser coffee in a filter. In either method water flows through the bed, leaching soluble coffee components from the grains. Any undissolved solids in the fluid are filtered from the extract as the liquid leaves the filter.

brewing technique hot water is poured over coffee grounds contained in a filter which is often conical in shape. The hot water flows down through the coffee bed under the influence of gravity, leaching soluble content. The only impediment to flow is the resistance provided by the porous bed and the filter. Figure 2.3b shows a schematic of the process. A drip filter machine is shown in figure 2.4. The drip filter brewing system was analysed by a group of applied mathematicians at the ESGI 87 study group with industry at the University of Limerick [10]. The problem was brought to the study group by coffee researchers at Philips Research in Eindhoven. Some of the aspects considered included the evolution of the shape of the coffee bed during brewing, correlations observed between the final bed shape and the quality of the brewed coffee and the use of a single jet or multiple jets (shower head) to deliver water to the coffee bed. Following this, a paper by one of the study group participants [64], analysed gravity driven flow in a conical filter, similar to that used in a drip filter machine, and constructed a mathematical model describing the flow. Since the inception of this study, some further publications have been released, mainly relating to the espresso brewing method. Ref. [18] investigates methods to estimate steady-state permeability of packed coffee beds. Using some simple model equations and statistical methods, ref. [60] investigates how some extraction variables might affect the quality of
espresso coffee. Despite the developments outlined above, there is an absence in the literature of a first principles model of coffee extraction which is validated by experiment. This study aims to address this deficit.

2.1.4 Current work

The material in this chapter is published in ref. [51]. The aim of this work is to formulate a comprehensive, experimentally validated, model of the physics of coffee extraction. The model should include the dissolution and transport of coffee within the coffee bed. It should also take into account the doubly porous nature of the coffee bed, which consists of pores between the coffee grains (intergranular), but also smaller pores within the coffee grains (intragranular). In this chapter, flow through a static, saturated coffee bed, under the influence of a pressure gradient is modelled using a double porosity model. The parameters in this macroscopic model are related to the microscopic properties of the coffee bed by an averaging procedure using Representative Elementary Volumes. This allows the model to be parametrised from experimentally measured microscopic quantities. Utilising multiscale modelling of extraction from coffee grains, we show that we can quantitatively model extraction from ground coffee in two situations: in a well stirred dilute suspension of coffee grains and in a packed coffee bed. In our model, extraction is divided into two regimes. In the first, a rapid extraction occurs from the surface of the coffee grains which yields the highest concentrations at any stage of the brewing process. In the second there is a slow extraction at lower concentrations from the interior of the grains. The model can be easily generalised to describe standard coffee brewing methods such as french press and drip filter coffee. It can also be extended to include unsaturated flow in the coffee bed.

We will begin by considering some coffee extraction experiments to motivate our models. The experiments presented here are a subset of a much large collec-
2.2 Coffee extraction experiments

A large number of experiments were carried out to investigate flow and extraction of coffee from coffee beds of various geometries. Two of these experiments will be outlined here and used to motivate the development of a mathematical model to replicate their results. The experiments were performed with a number of different coffee grinds.

2.2.1 Coffee grinds used

In the experiments presented here we make use of five different coffee grinds, ranging from a fine drip filter grind to a very coarse grind. The grind size distributions of these grinds are shown in figure 2.5. The first grind is a relatively fine grind, called Jacobs Krönung (JK) standard drip filter coffee grind. The next grinds used are the Douwe Egberts (DE) standard drip filter coffee grind and the Douwe Egberts coarse drip filter grind. Finally two further grinds were obtained by grinding Illy coffee beans using a Cimbali burr grinder. One very coarse grind was obtained using the #20 setting on the grinder. A second extremely coarse grind was obtained using the #30 setting on the grinder. The grind size distribution of the Cimbali #30 grind was too coarse to be analysed by the optical particle size analyzer used (Mastersizer 2000; Malvern Instruments Ltd, UK) and so is not included in figure 2.5. It is apparent from the graph that all distributions are bimodal, having two peaks. A first peak occurs at a particle size of 25–30 µm while the second peak occurs at a larger particle size and gradually shifts from left to right on the graph with the grind coarseness. The first peak accounts for...
single cell fragments: the cell size in coffee particles is 25–50 µm. The second peak accounts for particles comprising intact coffee cells. The grind size distribution is vitally important in coffee extraction, in that it affects both the fluid flow through the grind and the grind’s extraction kinetics.

![Grind size distributions of the coffee grinds used in experiments.](image)

**Figure 2.5:** Grind size distributions of the coffee grinds used in experiments.

The corresponding cumulative volume plot in figure 2.6 shows the cumulative volume of the distribution below a given value. Note that for JK drip filter grind almost 22% of the coffee bed volume is made up of particles with diameter less than 50 µm. This compares about 12% for the coarse Cimbali #20 grind. The high proportion of fine particles in the JK drip filter grind mean the grind distribution as a whole has a much higher surface area to volume ratio. This means the bed gives a much higher resistance to flow. Also the large volume represented by smaller particles should lead to a much faster extraction. If we assume the coffee particles are approximately spherical then we can convert the grind size distributions given in terms of volume fraction to number and surface area distributions. The distribution by mass is identical to the volume distribution (assuming constant particle density). We can also estimate quantities like the specific surface area of the grind distribution and equivalent spherical diameters.
2.2 Coffee extraction experiments

![Cumulative volume plot of the coffee grinds used in experiments.](image)

**Figure 2.6:** Cumulative volume plot of the coffee grinds used in experiments.

### 2.2.2 Maximum extractable solubles mass from coffee grind

Extraction from a coffee grain occurs following contact with water. However, not all of the coffee grain mass is soluble. Experiments conducted show that extractable mass of coffee grains in water at 90°C can range from 28% for very coarse grinds to 32% for very fine grinds. Equivalent experiments conducted at 21°C show reduced values of 23% for very coarse grinds and 27% for very fine grinds. These results were obtained using the fine and coarse grinds from Douwe Egberts (DE) coarse drip filter coffee. The extraction was carried out in glass beakers by continuously stirring the grind through the water with a magnetic stirrer for at least 5 hours to ensure maximum extraction. Increasing the extraction time from 5 hours to 10 hours did not change the extracted amount. Reduced extraction from larger coffee particles probably reflects the phenomenon that some solubles cannot be removed from closed cells inside the larger particle kernels. Coffee grains exposed to ambient humidity contain a certain amount of moisture which is absorbed in the grains. This moisture can be desorbed (together with other volatiles) by heating at 100°C in an oven. Subsequent exposure of dried coffee particles to atmospheric moisture at a relative humidity of 50% causes moisture re-sorption. It was found that 4–5% of the initial coffee mass can be removed through heating, but largely returns within 1–2 days after re-exposure to relative humidity of 50% at room temperature. The fact that the removal of volatile
material is observed to be mostly reversible indicates that the volatile material in coffee is predominately water and volatile organic compounds represent less than 1% of the coffee constituents by mass. Determining the maximum extractable solubles mass results, detailed above, is done by drying the coffee grains following extraction and comparing the initial and final masses. Adjustment is made for the initial moisture content in grains before extraction.

2.2.3 Coffee extraction kinetics during batch-wise brewing in a fixed water volume

The extraction kinetics of the five coffee grinds considered here were investigated by mixing 60 grams of coffee with a hot water volume, \( V_{\text{water}} = 0.5 \) litres, and measuring the concentration \( c_{\text{brew}} \) of extracted species as a function of time. The temperature of the liquid during extraction is 80–90°C. This was done by performing batch-wise extraction in a French-press type cylinder and using a piston to separate the brew from the grounds, after a certain extraction time, by pressing the mixture through a sheet of coffee filter paper on the cylinder bottom. The solubles concentration \( c_{\text{brew}} \) was subsequently determined by measuring the °Brix with a pocket refractometer (PAL-3, Atago, Japan). It was found for drip filter coffee that 1°Brix corresponds with \( c_{\text{brew}} = 8.25 \) g/litre. The latter calibration factor was obtained by evaporating all the water from the coffee brew and weighing the remaining non-volatile material. The resulting extraction profiles are shown in figure 2.7. This experiment clearly illustrates the key influence that the grind size distribution has on extraction.

2.2.4 Coffee extraction profiles from a cylindrical brewing chamber

A number of coffee extraction experiments were conducted with both a cylindrical brewing chamber and a conical Melitta filter. We will focus on the cylindrical brewing chamber here. In this setup, coffee is placed in a cylindrical flow-through cell and 1 litre of water at 90°C is forced through the coffee bed using a rotary vane pump. The system can operate in a constant flow mode with the pressure differential across the bed adjusting itself to the flow. Alternatively the pressure differential across the coffee bed can be fixed with the flow adjusting itself to
2.2 Coffee extraction experiments

Figure 2.7: Coffee solubles concentration profiles for different coffees and grind size distributions during batch extraction experiments. In these experiments 60 g of coffee with approximately 4% moisture was mixed with 0.51 of hot water in a French press type cylinder.

We make a number of observations based on the experimental data presented, which will be used to motivate the development of a mathematical model of the extraction process. Firstly, it is noted that the experiments tell us nothing about the filling stage, where the water initially infiltrates the dry coffee bed. To this end, it will be assumed that when the first coffee brew exits, the coffee bed, including the intragranular pores, is saturated with water. It is noted that in the case of the batch extraction experiment, in figure 2.7, the concentration of the coffee brew increases rapidly from zero to over half its maximum value at the beginning of extraction, before a much slower increase over a longer timescale towards its maximum value. This phenomena can also be seen in the cylindrical brewing chamber data in figure 2.8, where the concentration of the initial exiting brew is very high and this is maintained for a short time, before there is a large drop in the exiting concentration to a lower level and this gradually declines over
Figure 2.8: The coffee solubles concentration, measured in mg/gram, is plotted against mass of coffee beverage $M_{\text{brew}}$ (grams) for JK drip filter grind with a flow rate of 250 ml/min and pressure differential of 2.3 bar in (a) the coffee pot and (b) the beverage at filter exit, and for Cimbali #20 grind with a flow rate of 250 ml/min and pressure differential of 0.65 bar in (c) the coffee pot and (d) the beverage at filter exit. The mass of coffee used in both cases is 60 g including approximately 4% moisture. The brewing cylinder diameter is 59 mm. The coffee bed heights are 4.05 cm for JK drip filter grind and 5.26 cm for Cimbali #20 grind.

A longer period. This is consistent with the findings in ref. [72] where it was noted that extraction yield reached 90% of its final value within one minute. Large-sized roasted particles in the coffee grind feature a kernel comprising undamaged closed cells and a particle skin formed by damaged open cells. The grind distribution as seen in figure 2.5 also contains a significant proportion of fines or damaged cells. Thus the reason for the fast initial extraction may be due to reduced mass transfer resistances in the damaged particle skin and in the fines. The slow extraction may then be due to mass diffusion from intact cells in particle kernel. Thus the rate limiting step is diffusion from the particle kernel.

Some further experiments for JK standard drip filter grind are also useful for
2.2 Coffee extraction experiments

Figure 2.9: (a) Experimental setup for extraction from coffee flow-through-cell outlined in the text. (b) Experimental setup for gravity driven flow through a conical bed (not discussed in text).

The development here. These experiments consider different coffee bed masses and different values of absolute pressure in the bed. To compare results for coffee bed different masses (and hence different bed lengths) the extraction is performed for coffee bed masses of 12.5 g and 60 g. These masses correspond to bed depths of 1.12 cm and 4.05 cm respectively. The flow rate to the coffee bed is 250 ml/min in both cases. The pressure difference across the bed is measured in both cases. The solubles concentrations are measured in the coffee pot and at the filter exit. The results are shown in figure 2.10.

Figure 2.10: The coffee solubles concentration, measured in mg/gram, is plotted against mass of coffee beverage $M_{\text{brew}}$ (grams) for JK drip filter grind with a flow rate of 250 ml/min in (a) the coffee pot and (b) the beverage at filter exit for different coffee bed masses.
The influence of absolute pressure on extraction was also investigated by repeating the experiments in the coffee brewing cylinder at different values of absolute pressure but maintaining the same coffee bed mass and flow rate. In the case of JK standard drip filter grind, the absolute pressure in the brewing cylinder is increased from 2.3 bar to 9 bar. The resulting solubles concentrations profiles are plotted in figure 2.11. The results are seen to be virtually identical which indicates that the extraction kinetics are substantially independent of the absolute pressure (at least for the range of values considered) and that the results are reproducible to within a few percent. It also suggests that a possibly faster particle penetration with water at higher pressures does not substantially affect the observed extraction results.

![Figure 2.11: The coffee solubles concentration, measured in mg/gram, is plotted against mass of coffee beverage $M_{\text{brew}}$ (grams) for JK drip filter grind with a flow rate of 250 ml/min in (a) the coffee pot and (b) the beverage at filter exit for different values of absolute pressure in the brewing cylinder.](image)

2.3 Mathematical modelling

2.3.1 Basic modelling assumptions

It is assumed here that the coffee brewing process can be broken into three stages. Initially in the filling stage, hot water is poured on the dry coffee grounds and begins to fill the filter, but doesn’t leave. Next in the steady state stage the bed is saturated, water is still entering the bed, but also leaving at the same rate. In the last stage, the draining stage, no more water enters the bed but it still drains out. In the absence of experimental data to cover the other stages, only...
the steady state stage is considered here. However, the model developed can be
generalised to include the unsaturated flow, during the filling and draining stages.
In the steady state stage the coffee bed is considered as a static, saturated porous
medium with the flow driven by a pressure gradient. This pressure gradient may
be mechanically applied as in an espresso machine or hydrostatic as in a drip
filter machine. The bed is composed of a solid matrix of coffee grains which are
themselves porous. As the filling stage is not modelled here, initial conditions for
the steady state stage will have to be estimated or inferred from experimental
data. Furthermore any swelling of the coffee grains due to the addition of water
will not be modelled. It is assumed this swelling would occur during the filling
stage and would manifest itself in the steady state stage possibly as a slight shift
to the right of the grind size distribution. As discussed above, coffee is composed
of over 1800 different chemical compounds, but in this model we will just consider
a single entity and model coffee concentration or brew strength in line with the
experimental data shown. The model can of course be generalised to model the
concentration of any number of coffee constituents. Modelling a multicomponent
system such as coffee with a single component is a simplification and requires
some justification. Firstly, as mentioned in the introduction, relating taste to
the concentration of the different coffee components in a beverage is a non-trivial
matter; currently no ideal recipe exists. Apart from professional tasters, the
most widely used measure of coffee quality is the coffee brewing control chart.
This chart is recommended by both the Speciality Coffee Association of Europe
(SCAE) and the Speciality Coffee Association of America (SCAA). Given that the
most widely used measure of coffee quality considers coffee as a single component,
it seems logical to do so as well. Secondly, experiments carried out suggest that
many important coffee components have similar extraction kinetics as illustrated
in figure 2.12.

The structure of the coffee bed is central to the extraction process. It is
immediately obvious that the bed consists of two phases. Following ref. [9], the
highly permeable phase consisting of the pores between the coffee grains is called
the h-phase. The low permeability phase consisting of the coffee grains is called
the l-phase. At a microscopic level, there are two phases within the coffee grains.
The pore or void space within the grains is called the v-phase, while the solid coffee
cellular matrix is referred to as the s-phase. The coffee bed has three fundamental
length scales. The smallest of these is the size of the pores within the grains or
2. MATHEMATICAL MODELLING OF THE COFFEE BREWING PROCESS

Figure 2.12: Extraction experiments suggest that a large number of compounds found in coffee extract with similar kinetics [10].

the size of a coffee cell which may be 25–50µm. The average size of a coffee grain in the grind size distribution by volume, excluding single cell fragments, will be approximately an order of magnitude bigger. Finally the size (depth) of the coffee bed will typically be a few centimetres. In order to model the transport of coffee and water in the bed, conservation equations can be formed at each of these scales. On the microscale (cell size scale), conservation equations can be formed in the h-phase, v-phase and s-phase. At the intermediate (grain size) scale conservation equations can be formed in the h-phase and the l-phase. We refer to this as the mesoscale. At this scale an individual coffee grain is represented by two overlapping continua representing the void and solid phases within the grain. At the macroscale (coffee bed scale), the coffee bed is represented by three overlapping continua representing the h-phase, v-phase and s-phase. To reconcile the three representations, we can use the methods of homogenisation or volume averaging. Volume averaging will be adopted here. A schematic of the volume averaging process is shown in figure 2.13. This is very useful since it relates the averaged macroscopic quantities to the physical parameters at the microscale. Some macroscopic parameters may be measured by experiment, while others can be found from their averaged representation in terms of measurable microscopic quantities. The influence of microscale properties on the macroscale system parameters can be easily identified.
2.3 Mathematical modelling

Figure 2.13: Macroscale equations are matched to microscale equations using volume averaging. At a macroscopic level the system is represented by three overlapping continua for the intergranular pores (h-phase), intragranular pores (v-phase) and solid coffee (s-phase).

2.3.2 Coffee bed structure

2.3.3 Coffee bed description

The coffee bed is represented by a porous medium domain $\Omega_T$ with volume $V_T$. The domain can be split into an intergranular pores domain $\Omega_h$, with volume $V_h$ and a coffee grain domain $\Omega_l$, with volume $V_l$. $\Omega_l$ is further split into an intragranular pore domain $\Omega_v$, with volume $V_v$ and a solid coffee domain $\Omega_s$, with volume $V_s$. Clearly the equalities $V_h + V_l = V_T$ and $V_v + V_s = V_l$ hold. The following volume fractions are now defined

$$\phi_h = \frac{V_h}{V_T}, \quad \phi_l = \frac{V_l}{V_T}, \quad \phi_v = \frac{V_v}{V_l}, \quad \phi_s = \frac{V_s}{V_l}, \quad (2.3.1)$$

which leads to
\[ \phi_h + \phi_l = 1, \quad \phi_v + \phi_s = 1. \quad (2.3.2) \]

The concentrations (mass per unit volume) of coffee in the respective phases are \( c_h, c_v \) and \( c_s \). The vectors \( \mathbf{v}_h \) and \( \mathbf{v}_v \) denote the fluid velocity in the h-phase and v-phase respectively. The velocity of the solid will be denoted by \( \mathbf{v}_s \). The densities of the liquid solution in the respective phases are denoted by \( \rho_h \) and \( \rho_v \). Note that in general the liquid density will be dependent on the concentration of coffee solubles. The presentation in ref. [51] assumed a constant fluid density independent of concentration. The derivation here will be more general. Further notation will be introduced as required. The formulation of the equations presented here will follow refs. [9] and [33]. Since conservation equations will be formed at three different scales the variables at each scale will be denoted as macroscale (\( \tilde{\cdot} \)), mesoscale (\( \cdot^{*} \)) and microscale (\( \cdot \)) to avoid ambiguity.

### 2.3.3.1 Microscale point balance equations

The point balance equations for coffee and liquid within each of the phases on the microscale are

**h-phase**

\[
\frac{\partial c_h}{\partial t} = -\nabla \cdot (c_h \mathbf{v}_h + \mathbf{j}_h), \quad (2.3.3)
\]

\[
\frac{\partial \rho_h}{\partial t} = -\nabla \cdot (\rho_h \mathbf{v}_h). \quad (2.3.4)
\]

**v-phase**

\[
\frac{\partial c_v}{\partial t} = -\nabla \cdot (c_v \mathbf{v}_v + \mathbf{j}_v), \quad (2.3.5)
\]

\[
\frac{\partial \rho_v}{\partial t} = -\nabla \cdot (\rho_v \mathbf{v}_v). \quad (2.3.6)
\]

**s-phase**

\[
\frac{\partial c_s}{\partial t} = 0. \quad (2.3.7)
\]

The microscopic balance equations include the terms \( \mathbf{j}_h \) and \( \mathbf{j}_v \) which represent molecular diffusion of coffee solubles in the respective phases. Molecular diffu-
2.3 Mathematical modelling

sion in the solid phase is assumed negligible. We should note at this point that
rigorous application of volume averaging would require the specification of a well
defined closed system of equations at the microscale including the prescription of
boundary conditions at the interphase boundaries. Instead here we will use the
volume averaging procedure to motivate the macroscale equations, supplementing
the equations with constitutive equations where necessary to close the system.

2.3.3.2 Mesoscale point balance equations

The mesoscale balance equations are only required in the grains (l-phase) since
only two scales are needed in the h-phase. Thus the point balance equations for
coffee and liquid in the v-phase and the s-phase on the mesoscale are

\[ \frac{\partial}{\partial t} (\phi_v c_v^*) = - \nabla \cdot (\phi_v (c_v^* v_v^* + j_v^*)) - f_{v\rightarrow s}^*. \] (2.3.8)

\[ \frac{\partial}{\partial t} (\phi_v \rho_v^*) = - \nabla \cdot (\phi_v (\rho_v^* v_v^* + i_v^*)) - g_{v\rightarrow s}^*. \] (2.3.9)

\[ \frac{\partial}{\partial t} (\phi_s c_s^*) = - \nabla \cdot (\phi_s j_s^*) - f_{s\rightarrow v}^*. \] (2.3.10)

The terms \( f_{v\rightarrow s}^* \) and \( f_{s\rightarrow v}^* \) are source/sink terms representing transfer of coffee
solubles across the vs-interface and vice-versa. The term \( g_{v\rightarrow s}^* \) represents the
transfer of mass to the liquid as coffee solubles dissolve. The term \( i_v^* \) accounts
for any mechanical dispersion in the fluid velocity.

2.3.3.3 Macroscale point balance equations

For each phase, there are macroscopic point balance equations for mass of the
coffee and mass of liquid (flow equations). The solid is assumed stationary. The
macroscopic equations take the form:

\[ \frac{\partial}{\partial t} (\phi_h \bar{c}_h) = - \nabla \cdot (\phi_h (\bar{c}_h \bar{v}_h + \bar{j}_h)) - \bar{f}_{h\rightarrow l}. \] (2.3.11)

\[ \frac{\partial}{\partial t} (\phi_h \bar{\rho}_h) = - \nabla \cdot (\phi_h (\bar{\rho}_h \bar{v}_h + \bar{i}_h)) - \bar{g}_{h\rightarrow l}. \] (2.3.12)
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v-phase

\[ \frac{\partial}{\partial t}(\phi_l \phi_v \tilde{c}_v) = -\nabla \cdot (\phi_l \phi_v (\tilde{c}_v \tilde{v}_v + \tilde{j}_v)) - \tilde{f}_{v\rightarrow h} - \tilde{f}_{v\rightarrow s}, \]  
\[ (2.3.13) \]

\[ \frac{\partial}{\partial t}(\phi_l \phi_v \tilde{\rho}_v) = -\nabla \cdot (\phi_l \phi_v (\tilde{\rho}_v \tilde{v}_v + \tilde{i}_v)) - \tilde{g}_{v\rightarrow h} - \tilde{g}_{v\rightarrow s}, \]  
\[ (2.3.14) \]

s-phase

\[ \frac{\partial}{\partial t}(\phi_l \phi_s \tilde{c}_s) = -\nabla \cdot (\phi_l \phi_s \tilde{j}_s) - \tilde{f}_{s\rightarrow h} - \tilde{f}_{s\rightarrow v}. \]  
\[ (2.3.15) \]

\( \tilde{f}_{\alpha\rightarrow \beta} \) is transfer of coffee solubles from \( \alpha \)-phase to \( \beta \)-phase across \( \alpha\beta \) interface. Similarly \( \tilde{g}_{\alpha\rightarrow \beta} \) is transfer of mass in the coffee solution from \( \alpha \)-phase to \( \beta \)-phase across \( \alpha\beta \) interface.

2.3.4 Upscaling from microscale to macroscale

As mentioned above, the conservation equations at each of the scales can be related by representing the properties of the medium at a larger scale by averaging the properties at the smaller scale. This is useful to find the forms of the mass transfer terms in the macroscopic equation. An outline of the general upscaling procedure based on refs. [9, 33] and details of upscaling in this case are given in the next sections.

2.4 Volume averaging procedure

2.4.1 General upscaling procedure

The following procedure is mainly adapted from refs. [33] and [9]. In order to compare microscopic and macroscopic equations a procedure is needed for upscaling or averaging equations from a smaller scale to a larger scale. A general upscaling procedure from a microscopic scale to a macroscopic scale is outlined here.

Let the general form of a point balance equation for the concentration of a \( \gamma \)-species per unit volume of the \( \alpha \)-phase be

\[ \frac{\partial c_\alpha}{\partial t} = -\nabla \cdot (c_\alpha \mathbf{v}_\alpha + \mathbf{j}_\alpha) + G_\alpha, \]  
\[ (2.4.1) \]
where \( c_\alpha \) is the concentration of the \( \gamma \)-species, \( \mathbf{v}_\alpha \) is the fluid velocity in the \( \alpha \)-phase, \( \mathbf{j}_\alpha \) is the diffusive flux of the \( \gamma \)-species in the \( \alpha \)-phase, and \( G_\alpha \) is a source or sink of the \( \gamma \)-species in the \( \alpha \)-phase.

Let \( \beta \) represent all other phases in the porous medium. The \( \alpha \) subscript will be dropped where convenient. Equation 2.4.1 is the microscopic balance. The corresponding macroscopic balance equation is

\[
\frac{\partial}{\partial t}(\phi_\alpha c^*) = -\nabla \cdot (\phi_\alpha c^* \mathbf{v}^* + \phi_\alpha \mathbf{j}^*) + \phi_\alpha G^*,
\]  

where \( \phi_\alpha \) is the volume fraction of the \( \alpha \)-phase and the \( \cdot^* \) variables are macroscopic variables.

To relate (2.4.1) and (2.4.2), the averaged macroscale properties are defined by averaging (or integrating) (2.4.1) over an appropriate REV or Representative Elementary Volume. The length scale of an REV is much greater than the pore scale but much less than the full scale of the system. So if \( l \) is the length scale of an REV, \( d \) is the pore length scale and \( L \) is the full problem length scale then

\[
d \ll l \ll L.
\]  

The following notation is used

- The volume of an REV is \( \delta V \).
- The portion of the volume of an REV occupied by the \( \alpha \)-phase is \( \delta V^\alpha \).
- The union of the interfacial regions within the REV between the \( \alpha \)-phase and a \( \beta \)-phase is denoted \( S_{\alpha \beta} \).
- The unit vector normal to this surface oriented outward from the \( \alpha \)-phase is \( \mathbf{n}^\alpha \).

To average the microscopic balance equations two theorems, that transform the average of a derivative to the derivative of an average, are needed. The time averaging theorem is given by

\[
\int_{\delta V} \frac{\partial F}{\partial t} dV = \frac{\partial}{\partial t} \int_{\delta V} F dV - \sum_{\beta \neq \alpha} \int_{S_{\alpha \beta}} \mathbf{n}^\alpha \cdot \mathbf{w}_b F|_\alpha dS,
\]

where \( F \) is some scalar field property of the microscale and \( F|_\alpha \) just indicates that the microscale property \( F \) in the \( \alpha \)-phase is being integrated over the \( \alpha \beta \)-interface.
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\( w_b \) is the velocity of \( S_{\alpha\beta} \). The summation \( \sum_{\beta \neq \alpha} \) just denotes a summation over all phases except the \( \alpha \)-phase.

The divergence averaging theorem is given by

\[
\int_{\delta V} \nabla \cdot \mathbf{B} dV = \nabla \cdot \int_{\delta V} \mathbf{B} dV + \sum_{\beta \neq \alpha} n^\alpha \cdot \mathbf{B}|_{\alpha} dS, \quad (2.4.5)
\]

where \( \mathbf{B} \) is some vector field property of the microscale and \( \mathbf{B}|_{\alpha} \) just indicates that \( \mathbf{B} \) is being integrated over the \( \alpha\beta \)-interface. The summation \( \sum_{\beta \neq \alpha} \) just denotes a summation over all phases except the \( \alpha \)-phase.

Next some phase averages are defined:

The Intrinsic Phase Average of a quantity \( F \) over the \( \alpha \)-phase is defined by:

\[
\langle F \rangle^\alpha = \overline{F}^\alpha = \frac{1}{\delta V^\alpha} \int_{\delta V^\alpha} F dV. \quad (2.4.6)
\]

The Phase Average of a quantity \( F \) over the \( \alpha \)-phase is defined by:

\[
\langle F \rangle = \overline{F} = \frac{1}{\delta V} \int_{\delta V} F dV = \phi_\alpha \overline{F}^\alpha. \quad (2.4.7)
\]

The Mass Weighted Average of a quantity \( F \) over the \( \alpha \)-phase is defined by:

\[
\langle F' \rangle^\alpha = \overline{F'}^\alpha = \frac{1}{\langle \rho \rangle^\alpha} \int_{\delta V^\alpha} \rho F dV = \frac{\langle \rho F \rangle^\alpha}{\langle \rho \rangle^\alpha}. \quad (2.4.8)
\]

It will also be necessary to be able to write the average of a product of the form \( \langle c v \rangle^\alpha \) in terms of the individual averages \( \langle c \rangle^\alpha \) and \( \langle v \rangle^\alpha \). To do this consider the following:

- Let \( \hat{v} = v - \langle v \rangle^\alpha \) be the deviation of the true velocity from the mean velocity.

- Let \( \hat{c} = c - \langle c \rangle^\alpha \) be the deviation of the true concentration from the mean concentration.

Then

\[
\langle \hat{v} \rangle^\alpha = \langle v - \langle v \rangle^\alpha \rangle^\alpha = \langle v \rangle^\alpha - \langle v \rangle^\alpha = 0, \quad (2.4.9)
\]

\[
\langle \hat{c} \rangle^\alpha = \langle c - \langle c \rangle^\alpha \rangle^\alpha = \langle c \rangle^\alpha - \langle c \rangle^\alpha = 0. \quad (2.4.10)
\]
Thus

\[ \langle cv \rangle^\alpha = \langle (\langle c \rangle^\alpha + \dot{c})(\langle v \rangle^\alpha + \dot{v}) \rangle^\alpha \]
\[ = \langle c \rangle^\alpha \langle v \rangle^\alpha + \langle \dot{c} \dot{v} \rangle^\alpha + \langle \dot{c} \rangle^\alpha \langle v \rangle^\alpha + \langle c \rangle^\alpha \langle \dot{v} \rangle^\alpha \]
\[ = \langle c \rangle^\alpha \langle v \rangle^\alpha + \langle \dot{c} \dot{v} \rangle^\alpha . \quad (2.4.11) \]

The term \( \langle \dot{c} \dot{v} \rangle^\alpha \) is called the dispersive flux.

Now the averaging process can be performed. Firstly (2.4.1) integrated over \( \delta V^\alpha \) yields

\[ \int_{\delta V^\alpha} \frac{\partial c}{\partial t} dV = - \int_{\delta V^\alpha} \nabla \cdot (cv + j) dV + \int_{\delta V^\alpha} G dV. \quad (2.4.12) \]

Now applying theorems (2.4.4) and (2.4.5) yields

\[ \frac{\partial}{\partial t} \int_{\delta V^\alpha} c dV = - \nabla \cdot \left( \int_{\delta V^\alpha} (cv + j) dV \right) \]
\[ - \sum_{\beta \neq \alpha} \int_{S_{\alpha \beta}} n^\alpha \cdot (c(v - w_b) + j) |_a dS \]
\[ + \int_{\delta V^\alpha} G dV. \quad (2.4.13) \]

This can be written in terms of averaged quantities by dividing across by \( \delta V = \frac{\delta V^\alpha}{\phi_a} \) to give

\[ \frac{\partial}{\partial t} (\phi_a \langle c \rangle^\alpha) = - \nabla \cdot \phi_a (\langle cv \rangle^\alpha + \langle j \rangle^\alpha) \]
\[ - \frac{1}{\delta V} \sum_{\beta \neq \alpha} \int_{S_{\alpha \beta}} n^\alpha \cdot (c(v - w_b) + j) |_a dS \]
\[ + \phi_a \langle G \rangle^\alpha . \quad (2.4.14) \]

Utilising the formula for the average of a product, it can be seen that
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\[
\begin{align*}
\frac{\partial}{\partial t} (\phi_\alpha \langle c \rangle^\alpha) &= - \nabla \cdot \phi_\alpha (\langle c \rangle^\alpha \langle v \rangle^\alpha + \langle \dot{c} \rangle^\alpha + \langle j \rangle^\alpha) \\
&\quad - \frac{1}{\delta V} \sum_{\beta \neq \alpha} \int_{S_{\alpha\beta}} n_\alpha \cdot \left( c(v - w_b) + j \right)_{\alpha} dS \\
&\quad + \phi_\alpha \langle G \rangle^\alpha.
\end{align*}
\]

Comparing this to the macroscopic point balance equation \((2.4.2)\) gives the following relations between the macroscopic and microscopic quantities

\[
\begin{align*}
c^* &= \langle c \rangle^\alpha, \\
v^* &= \langle v \rangle^\alpha, \\
j^* &= \langle \dot{c} \rangle^\alpha + \langle j \rangle^\alpha, \\
\phi_\alpha G^* &= \phi_\alpha \langle G \rangle^\alpha \\
&\quad + \frac{1}{\delta V} \sum_{\beta \neq \alpha} \int_{S_{\alpha\beta}} n_\alpha \cdot \left( c(v - w_b) + j \right)_{\alpha} dS.
\end{align*}
\]

It can be seen that the microscale convection and diffusion processes at the interfaces are source terms for the macroscopic equation. Also the macroscopic diffusive flux is the sum of the averaged microscopic diffusive flux and the dispersive flux.

2.5 Upscaling from microscale to macroscale equations

The upscaling process basically involves choosing an REV (Representative Elementary Volume) around every point on the larger scale and representing the properties of the medium by the averaged properties of the smaller scale over the REV. For these purposes suitable averages need to be defined including a phase average and an intrinsic phase average. Also needed are a time averaging theorem and a divergence averaging theorem. An outline of the upscaling procedure used here has been given in section \([2.4.1]\). Before continuing some notes on the REVs being used are necessary. Two different REVs will be used. One will have a scale between that of a coffee cell and a coffee grain. The second will have a scale
2.5 Upscaling from microscale to macroscale equations

between that of a coffee grain and the coffee bed. For the REVs the following notation is used.

\( V_1 \): Volume of the smaller REV.

\( V_{1s} \): Volume of solid in the smaller REV.

\( V_{1v} \): Volume of void space in smaller REV.

\( V_0 \): Volume of larger REV.

\( V_{0l} \): Volume of grains (l-phase) in larger REV.

\( V_{0h} \): Volume of void space (h-phase) in larger REV.

Also due to the properties of an REV

\[
\begin{align*}
\phi_h &= \frac{V_{0h}}{V_0} = \frac{V_h}{V_T}, \\
\phi_v &= \frac{V_{1v}}{V_1} = \frac{V_v}{V_l}, \\
\phi_s &= \frac{V_{1s}}{V_1} = \frac{V_s}{V_l}.
\end{align*}
\]  

(2.5.1)

(2.5.2)

2.5.1 Equations for upscaling

We start with the microscale point balance equations (2.3.3)–(2.3.7) and upscale to the macroscale point balance equations (2.3.11)–(2.3.15).

2.5.2 Upscaling in l-phase: microscale to mesoscale

2.5.2.1 Conservation of coffee in v-phase

The averaged form of the microscopic point balance equation (2.3.5) over the smaller REV is

\[
\frac{\partial}{\partial t} \left( \phi_v \langle c_v \rangle^v \right) = -\nabla \cdot \phi_v \left( \langle c_v \rangle^v \langle \mathbf{v}_v \rangle^v + \langle \hat{c}_v \mathbf{v}_v \rangle^v + \langle \mathbf{j}_v \rangle^v \right) \\
- \frac{1}{V_1} \int_{S_{vs}} \mathbf{n}^v \cdot \left( c_v (\mathbf{v}_v - \mathbf{w}_{vs}) + \mathbf{j}_v \right) dS.
\]  

(2.5.3)
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At this point in ref. [51], it was assumed that the surface $S_{vs}$ is a material surface so $v_{-w_{vs}} = 0$. We do not make this assumption here. Comparing the averaged form with the mesoscale form in (2.3.8) it can be seen that

$$c^*_v = \langle c_v \rangle^v,$$  \hspace{1cm} (2.5.4)
$$v^*_v = \langle v_v \rangle^v,$$  \hspace{1cm} (2.5.5)
$$j^*_v = \langle  \dot{c}_v \nu_v \rangle^v + \langle j_v \rangle^v,$$  \hspace{1cm} (2.5.6)
$$f^*_{v \rightarrow s} = \frac{1}{V_1} \int_{S_{vs}} n^v \cdot (c_v (v_v - w_{vs}) + j_v) dS.$$

(2.5.7)

### 2.5.2.2 Conservation of liquid in $v$-phase

The averaged form of the microscopic point balance equation (2.3.6) over the smaller REV is

$$\frac{\partial}{\partial t} (\phi_v \langle \rho_v \rangle^v) = - \nabla \cdot \phi_v (\langle \rho_v \rangle^v v_v + \langle \dot{\rho}_v \nu_v \rangle^v)$$
$$- \frac{1}{V_1} \int_{S_{vs}} n^v \cdot (\rho_v (v_v - w_{vs})) dS.$$

(2.5.8)

Again we do not assume the surface $S_{vs}$ is a material surface and so we get a source term from the $s$-phase $g^*_{v \rightarrow s}$. Comparing this averaged form with the mesoscale form in (2.3.9) it can be seen that

$$\rho^*_v = \langle \rho_v \rangle^v,$$  \hspace{1cm} (2.5.9)
$$v^*_v = \langle v_v \rangle^v,$$  \hspace{1cm} (2.5.10)
$$i^*_v = \langle \dot{\rho}_v \nu_v \rangle^v,$$  \hspace{1cm} (2.5.11)
$$g^*_{v \rightarrow s} = \frac{1}{V_1} \int_{S_{vs}} n^v \cdot (\rho_v (v_v - w_{vs})) dS.$$

(2.5.12)
2.5 Upscaling from microscale to macroscale equations

2.5.2.3 Conservation of coffee solid in s-phase

The averaged form of the microscopic point balance equation (2.3.7) over the smaller REV is

$$\frac{\partial}{\partial t}(\phi_s \langle c_s \rangle_s) = -\frac{1}{V_1} \int_{S_{sv}} n^s \cdot (-c_s w_{sv}) dS.$$  \hspace{1cm} (2.5.13)

Comparing this averaged form with the mesoscale form in (2.3.10) it can be seen that

$$c_s^* = \langle c_s \rangle^s,$$ \hspace{1cm} (2.5.14)
$$v_s^* = 0,$$ \hspace{1cm} (2.5.15)
$$f_{s\rightarrow v}^* = \frac{1}{V_1} \int_{S_{sv}} n^s \cdot (-c_s w_{sv}) dS.$$ \hspace{1cm} (2.5.16)

2.5.3 Upscaling to macroscale

2.5.3.1 Conservation of coffee in h-phase

The averaged form of the microscopic point balance equation (2.3.3) over the larger REV is

$$\frac{\partial}{\partial t}(\phi_h \langle c_h \rangle^h) = -\nabla \cdot \phi_h (\langle c_h \rangle^h (v_h)^h + \langle \dot{c}_h \dot{v}_h \rangle^h + \langle j_h \rangle^h)$$
$$-\frac{1}{V_0} \int_{S_{hl}} n^h \cdot (c_h (v_h - w_{hl}) + j_h) dS.$$ \hspace{1cm} (2.5.17)

Comparing this averaged form with the macroscale form in (2.3.11) it can be seen that

$$\tilde{c}_h = \langle c_h \rangle^h,$$ \hspace{1cm} (2.5.18)
$$\tilde{v}_h = \langle v_h \rangle^h,$$ \hspace{1cm} (2.5.19)
$$\tilde{j}_h = \langle c_h \dot{v}_h \rangle^h + \langle j_h \rangle^h,$$ \hspace{1cm} (2.5.20)
$$\tilde{f}_{h \rightarrow l} = \frac{1}{V_0} \int_{S_{hl}} n^h \cdot (c_h (v_h - w_{hl}) + j_h) dS.$$ \hspace{1cm} (2.5.21)
Here $S_{hl}$ is the effective surface between the h-phase and the l-phase and includes boundaries between the h-phase and the v-phase and the h-phase and the s-phase.

### 2.5.3.2 Conservation of liquid in h-phase

The averaged form of the microscopic point balance equation (2.3.4) over the larger REV is

$$\frac{\partial}{\partial t} \langle \rho_h \rangle^h = - \nabla \cdot \phi_h (\langle \rho_h \rangle^h \langle v_h \rangle^h + \langle \rho_h \tilde{v}_h \rangle^h) \tag{2.5.22}$$

Comparing this averaged form with the macroscale form in (2.3.12) it can be seen that

$$\tilde{\rho}_h = \langle \rho_h \rangle^h \tag{2.5.23}$$
$$\tilde{v}_h = \langle v_h \rangle^h \tag{2.5.24}$$
$$\tilde{i}_h = \langle \rho_h \tilde{v}_h \rangle^h \tag{2.5.25}$$
$$\tilde{g}_{h \rightarrow l} = \frac{1}{V_0} \int_{S_{hl}} n^h \cdot (\rho_h (v_h - w_{hl})) dS. \tag{2.5.26}$$

### 2.5.3.3 Conservation of coffee in v-phase

The averaged form of the microscopic point balance equation (2.3.8) over the larger REV is

$$\frac{\partial}{\partial t} (\phi_v \langle c_v^* \rangle^l) = - \nabla \cdot \phi_v (\langle c_v^* \rangle^l \langle v_v^* \rangle^l + \langle c_v^* \tilde{v}_v^* \rangle^l + \langle j_v^* \rangle^l) \tag{2.5.27}$$

Comparing this averaged form with the macroscale form in (2.3.13) it can be seen that
\[ \tilde{c}_h = \langle c_v^* \rangle^l = \langle (c_v)^v \rangle^l, \]  

(2.5.28)

\[ \tilde{v}_v = \langle v_v^* \rangle^l = \langle (v_v)^v \rangle^l, \]  

(2.5.29)

\[ \tilde{j}_v = \langle j_v^* \rangle^l + \langle c_v^* v_v^* \rangle^l \]  

(2.5.30)

\[ \tilde{f}_v \rightarrow h = \frac{\phi_v}{V_0} \int_{S_{lh}} n^l \cdot (\langle c_v \rangle^v (\langle v_v \rangle^v - w_{lh}) + \langle j_v \rangle^v) dS, \]  

(2.5.31)

\[ \tilde{f}_v \rightarrow s = \frac{\phi_l}{V_0} \left( \frac{1}{V_1} \int_{S_{vs}} n^v \cdot (c_v (v_v - w_{vs}) + j_v) dS \right) dV_0. \]  

(2.5.32)

It will be later assumed that \[ \tilde{v}_v = 0 \] and \[ \tilde{j}_v = 0 \] but of course it will still be possible to have \[ v_v^* \neq 0 \] and \[ j_v^* \neq 0. \]

### 2.5.3.4 Conservation of liquid in v-phase

The averaged form of the microscopic point balance equation (2.3.9) over the larger REV is

\[ \frac{\partial}{\partial t} \left( \phi_l \phi_v \langle \rho_v^* \rangle^l \right) = -\nabla \cdot \phi_l \phi_v (\langle \rho_v^* \rangle^l \langle v_v^* \rangle^l + \langle j_v^* \rangle^l + \langle i_v^* \rangle^l) \]  

\[ - \frac{\phi_v}{V_0} \int_{S_{lh}} n^l \cdot (\rho_v^* (v_v - w_{lh}) + i_v^*) dS \]  

(2.5.33)

\[ - \phi_l \langle g_v^{*r} \rangle^l. \]  

(2.5.34)

Comparing this averaged form with the macroscale form in (2.3.14) it can be seen that
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\[ \tilde{\rho}_h = \langle \rho^s_h \rangle^l = \langle \langle \rho_v \rangle^v \rangle^l, \]  
(2.5.35)

\[ \tilde{\mathbf{v}}_v = \langle \mathbf{v}^s_v \rangle^l = \langle \langle \mathbf{v}_v \rangle^v \rangle^l, \]  
(2.5.36)

\[ \tilde{\mathbf{i}}_v = \langle \mathbf{i}^s_v \rangle^l + \langle \hat{\rho}^v \hat{\mathbf{v}}^s_v \rangle^l \]  
= \langle \langle \mathbf{i}_v \rangle^v \rangle^l + \langle \hat{\rho}^v \hat{\mathbf{v}}^s_v \rangle^l, \]  
(2.5.37)

\[ \tilde{g}_{v \rightarrow h} = \frac{\phi_v}{V_0} \int_{S_{ih}} \mathbf{n}^1 \cdot (\langle \rho_v \rangle^v (\langle \mathbf{v}_v \rangle^v - \mathbf{w}_{lh}) + \langle \mathbf{i}_v \rangle^v) dS, \]  
(2.5.38)

\[ \tilde{g}_{v \rightarrow s} = \phi_l \langle g^*_{v \rightarrow s} \rangle^l = \frac{1}{V_0} \int_{V_0} \left( \frac{1}{V_1} \int_{S_{sv}} \mathbf{n}^v \cdot (\rho_v (\mathbf{v}_v - \mathbf{w}_{vs})) dS \right) dV_0. \]  
(2.5.39)

2.5.3.5 Conservation of coffee in s-phase

The averaged form of the microscopic point balance equation (2.3.10) over the larger REV is

\[ \frac{\partial}{\partial t} (\phi_l \phi_s \langle c^s_s \rangle^l) = -\nabla \cdot \phi_l \phi_s (\langle \mathbf{j}^s_s \rangle^l) \]  
- \frac{\phi_s}{V_0} \int_{S_{ih}} \mathbf{n}^1 \cdot (\langle c^s_s \rangle^s (-\mathbf{w}_{lh}) + \langle \mathbf{j}^s_s \rangle^s) dS

\[ = -\phi_l \langle \mathbf{f}^*_{s \rightarrow v} \rangle^l. \]  
(2.5.40)

Comparing this averaged form with the macroscale form in (2.3.15) it can be seen that

\[ \tilde{c} = \langle c^s_s \rangle^l = \langle \langle c^s_s \rangle^s \rangle^l, \]  
(2.5.41)

\[ \tilde{\mathbf{v}}_s = \mathbf{0}, \]  
(2.5.42)

\[ \tilde{\mathbf{j}}_s = \langle \mathbf{j}^s_s \rangle^l = \langle \langle c^s_s \rangle^s \rangle^l = \mathbf{0}, \]  
(2.5.43)

\[ \tilde{f}_{s \rightarrow h} = \frac{\phi_s}{V_0} \int_{S_{ih}} \mathbf{n}^1 \cdot (\langle c^s_s \rangle^s (-\mathbf{w}_{lh})) dS, \]  
(2.5.44)

\[ \tilde{f}_{s \rightarrow v} = \phi_l \langle f^*_{s \rightarrow v} \rangle^l \]  
\[ = \frac{1}{V_0} \int_{V_0} \left( \frac{1}{V_1} \int_{S_{sv}} \mathbf{n}^s \cdot (-c^s_s \mathbf{w}_{lh}) dS \right) dV_0. \]  
(2.5.45)
2.6 Developing macroscale equations

The macroscopic balance equations in section 2.3.3.3 are in a quite general form. Some assumptions have already been made, but in order to simplify things we make some further assumptions. We also need to introduce terms to model the transport of fluid and coffee within the bed. To begin we consider continuity of flux at the interphase boundaries. A key question is how to represent the dissolution of coffee into the interstitial liquid and in particular to determine how this influences the density of the coffee solution. There are four options to model the addition of coffee solubles to the coffee liquid solution:

1. Assume the liquid volume stays fixed and that added coffee solute increases the liquid density. In this case the dissolution of coffee in the intragranular pores should draw liquid into the pores to fill the volume created by the dissolved coffee.

2. Assume that the liquid density stays fixed, but the added coffee solute increases the liquid volume. As the coffee solid density is higher than the coffee solution this process would ‘push’ liquid out of the intragranular pores.

3. Assume both the coffee solution density and volume change due to the addition of coffee solubles. In this case the relationship between the solution density and the coffee solute concentration must be specified as \( \rho = \rho(c) \). For example \( \rho = \text{constant} \) corresponds to 2 while \( \rho = \rho_w + c \) corresponds to 1. Here \( \rho_w \) is the water density in the liquid solution. More generally equations of state of a fluid can depend on pressure, temperature as well as concentrations of its constituent components. This is discussed in detail in ref. [8].

4. The final possibility if that we assume that neither the density or volume of the liquid is changed by the added solute mass. This is of course incorrect as mass may not be conserved, but may be reasonably accurate in the limit of low solute concentrations. In this case solute concentration evolution can be tracked separately and assumed independent of the liquid solution properties.
2. MATHEMATICAL MODELLING OF THE COFFEE BREWING PROCESS

For the development here we assume that the density of the liquid is constant and does not change with coffee concentration. This is consistent with ref. [54] where it is noted that the material extracted from coffee has little influence on liquid density, although it does increase it somewhat. Thus $\tilde{\rho}_h = \tilde{\rho}_v = \rho$. We also assume initially that the liquid volume does not change with the addition of coffee solute although we will neglect this later. This means that we must account for suction of liquid into the grains to fill the space created by dissolving coffee. Under these assumptions our continuity of flux equations become:

$$\tilde{g}_{h \rightarrow t} = -\tilde{g}_{v \rightarrow h}, \quad (2.6.1)$$
$$\tilde{f}_{h \rightarrow t} = -\tilde{f}_{v \rightarrow h} - \tilde{f}_{s \rightarrow h}, \quad (2.6.2)$$
$$\tilde{g}_{v \rightarrow s} = 0, \quad (2.6.3)$$
$$\tilde{f}_{v \rightarrow s} = -\tilde{f}_{s \rightarrow v}. \quad (2.6.4)$$

Note again, we have neglected the influence of the solute concentration on the liquid solution density. It is also assumed that no transport occurs within the $l$-phase on the macroscale. This simply means that liquid or coffee does not transport directly from grain to grain within the bed. Any mechanical dispersion in the flow in the $h$-phase is not considered. Thus the five macroscopic equations reduce to the following

$$\frac{\partial}{\partial t}(\phi_h \tilde{c}_h) = -\nabla \cdot (\phi_h (\tilde{c}_h \tilde{v}_h + \tilde{j}_h)) + \tilde{f}_{v \rightarrow h} + \tilde{f}_{s \rightarrow h}, \quad (2.6.5)$$
$$\rho \frac{\partial \phi_h}{\partial t} = -\rho \nabla \cdot (\phi_h \tilde{v}_h) - \tilde{g}_{h \rightarrow t}, \quad (2.6.6)$$
$$\frac{\partial}{\partial t}(\phi_l \phi_v \tilde{c}_v) = -\tilde{f}_{v \rightarrow h} + \tilde{f}_{s \rightarrow v}, \quad (2.6.7)$$
$$\rho \frac{\partial}{\partial t}(\phi_l \phi_v) = +\tilde{g}_{h \rightarrow t}, \quad (2.6.8)$$
$$\frac{\partial}{\partial t}(\phi_l \phi_s \tilde{c}_s) = -\tilde{f}_{s \rightarrow h} - \tilde{f}_{s \rightarrow v}. \quad (2.6.9)$$

It is important to clarify some of the modelling details at this point. As it stands, we do not have a closed system of equations. We have six variables $\phi_h$, $\tilde{c}_h$, $\tilde{v}_h$, $\phi_v$, $\tilde{c}_v$ and $\tilde{c}_s$ and five equations. To close the system we will make some assumptions on the nature of the solute extraction, in the absence of a better understanding of extraction at the grain scale. In its current form, dissolution of coffee can be
reflected in an increase of intergranular porosity $\phi_h$ or intragranular porosity $\phi_v$ or a decrease in solid density $\tilde{c}_s$. When the coffee mass transfer terms $\tilde{f}_{v\rightarrow h}$, $\tilde{f}_{s\rightarrow v}$ and $\tilde{f}_{s\rightarrow h}$ are specified in terms of the system variables, we will assume $\phi_h$ and $\tilde{c}_s$ are constant and dissolution of coffee is completely reflected in an increase in $\phi_v$. This means we will have one less variable than equations, but an extra variable will be introduced to describe transfer of liquid to the grains in response to increasing $\phi_v$. Expressions to model the fluid velocity $\tilde{v}_h$, the total macroscopic flux $\tilde{j}_h$, the fluid mass transfer term $\tilde{g}_{h\rightarrow l}$ also need to be specified. The main transfers occurring in the coffee bed are shown in figure 2.14.

![Figure 2.14: Mass transfers occurring in the coffee bed.](image)

### 2.6.1 Fluid velocity

Darcy’s Law allows us to relate an averaged velocity or discharge in the pores to the pressure gradient. The relations in the h-phase are given by

$$
\tilde{u}_h = \phi_h \tilde{v}_h, \quad \tilde{u}_h = -\frac{\tilde{k}_h}{\mu} (\nabla \tilde{p}_h + \rho g), \quad \tilde{k}_h = \tilde{k}_h(\phi_h),
$$

where $\tilde{p}_h$ is the macroscopic pressure gradient in the h-phase, $\tilde{k}_h$ is the permeability and $\mu$ is the viscosity of water. While it is not presented here, Darcy’s law can be derived by averaging the microscale equation for balance of linear momentum.
of the fluid. This averaging procedure can be found either via volume averaging or homogenisation in refs. [8, 9, 45]. The following assumptions are made during the averaging process [9]:

- The fluid is Newtonian.
- Inertial forces are negligible relative to viscous ones.
- The effect of momentum transfer within the fluid as a result of velocity gradients is negligible compared to the drag induced by the fluid-solid interface.

### 2.6.2 Total macroscopic flux

The total macroscopic flux, \( \tilde{j}_h \), is made up of the macroscopic average of molecular diffusion \( j_h^a \) and the dispersive flux \( j_h^b \):

\[
\tilde{j}_h = \langle j_h \rangle^h + \langle \hat{c}_h \hat{\nabla}h \rangle^h = j_h^a + j_h^b. \quad (2.6.11)
\]

The microscopic diffusive flux can be represented by Fick’s Law:

\[
j_h = -D \nabla c_h, \quad (2.6.12)
\]

where \( D \) is the diffusion coefficient of the species in water. The macroscopic equivalent is obtained by averaging this expression and will generally depend on the structure of the porous medium. This average is represented by

\[
j_h^a = -D \tilde{T}^a(\phi) \cdot \nabla \tilde{c}_h = -D^a(\phi) \cdot \nabla \tilde{c}_h. \quad (2.6.13)
\]

where the \( \tilde{\cdot} \) here on \( \tilde{T}^a \) means this is a tensor of rank two which represents the tortuosity of the porous medium. For an isotropic porous medium this can be adjusted to

\[
j_h^a = -\frac{D}{\tau} \nabla \tilde{c}_h, \quad (2.6.14)
\]

where \( \tau \) is the tortuosity defined by

\[
\tau = \frac{L_e}{L} = \frac{\text{actual path length}}{\text{macroscopic path length}}. \quad (2.6.15)
\]

The tortuosity must be estimated in terms of the porosity. Various functional relationships are used in the literature. Some of these include
2.6 Developing macroscale equations

\[ \tau = \phi^{-\frac{1}{3}}, \quad \tau = \phi^{-\frac{1}{2}}, \quad \tau = \frac{1}{1 - \alpha(1 - \phi)}. \quad (2.6.16) \]

In the final expression \( \alpha = \frac{r^3}{v} \) is a shape factor with \( r \) being the object radius, \( \sigma \) being the object cross sectional area and \( V \) being the object volume. Thus for spheres for example \( \alpha = 0.75 \). In this case the first expression from ref. [46] will be adopted. The other expressions and tortuosity in general is discussed in ref. [56]. Thus macroscopic diffusion is approximated by

\[ j^h_a = -D \nabla \bar{c}_h = -\phi^\frac{1}{3}D \nabla \bar{c}_h. \quad (2.6.17) \]

2.6.3 Dispersive flux

Dispersion occurs due to variations in the microscopic velocity of the phase with respect to the averaged velocity, and molecular diffusion [9]. Thus molecular diffusion contributes to the dispersive flux in addition to the diffusive flux at the macroscopic level. In general the dispersive flux is given by

\[ j^b_h = \langle \dot{c}_h \dot{v}_h \rangle^h = -\bar{D} \cdot \nabla \bar{c}_h, \quad (2.6.18) \]

where \( \bar{D} \) is a rank 2 tensor called the dispersion tensor. \( \bar{D} \) is both positive definite and symmetric. One commonly used expression is

\[ D_{ij} = a_{ijkl} \frac{v_k v_l}{v}, \quad (2.6.19) \]

where \( a_{ijkl} \) is a fourth order tensor and \( v_i = \langle v_i \rangle^h \) is the average velocity in the \( i \)-th direction and \( v = |v| \) where \( v \) is the average velocity vector in this instance. For an isotropic porous medium the following expression is often used:

\[ D_{ij} = \left( a_T \delta_{ij} + (a_L - a_T) \frac{v_i v_j}{v^2} \right) v. \quad (2.6.20) \]

The coefficients \( a_L \) and \( a_T \) here are the longitudinal and transverse dispersivities of the porous medium. For a phase that completely fills a pore space, \( a_L \) is a length that should be of the same order of the pore size. \( \delta_{ij} \) is the Kronecker delta. Also it is required that

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2.6.4 Coffee mass transfer terms

Experimental results in section 2.2 suggest that there are two fundamental extraction mechanisms from the coffee grains. A rapid extraction from fines (single cells fragments) and damaged cells on the surface of larger particles and a slower extraction from the kernels of larger particles. Various different models have been applied to represent such situations, particularly in the area of supercritical fluids. The main models are reviewed in ref. [53]. These models include linear driving force, bi-linear driving force, shrinking core, broken plus intact cells in series, broken plus intact cells in parallel and a combined broken plus intact cells with shrinking core model. These models are widely used in modelling extraction with supercritical fluids and have been considered in a number of papers, both theoretical and experimental, including refs. [32, 35, 42, 69]. In ref. [35], it is noted that the broken plus intact cell model typically features an initial constant extraction period dominated by extraction from the broken cells, then a falling extraction rate period as broken cells on the surface are depleted and finally a diffusion controlled period dominated by extraction from the intact cells. These general features are evident in the extraction experiments in section 2.2. The models used here are quite similar to the broken plus intact cells in parallel. The extraction term \( \tilde{f}_{v \rightarrow h} \) is transfer from the intragranular pores in the grains to the intergranular pores and is similar to extraction from intact cells. The term \( \tilde{f}_{s \rightarrow h} \) is direct extraction from the solid grain matrix surface into the intergranular pores and is similar to extraction from the broken cells. The term \( \tilde{f}_{s \rightarrow v} \) models dissolution of coffee solubles from the cell walls into the intragranular pores.

It is necessary to estimate these mass transfer terms of the general form \( f_{\alpha \rightarrow \beta} \), which govern the transfer of solute from the solid phase to the liquid phase both within the grains and from the surface of the grains. It is also necessary to estimate the mass transfer of solute from liquid within the grains to liquid in the pores between the grains. This subject is dealt with from a food processing and engineering standpoint in ref. [2]. More general and technical developments are
2.6 Developing macroscale equations

found in refs. [9] and [19]. The transfer term $f_{\alpha \rightarrow \beta}$ may be due to a number of processes. Some typical examples are adsorption (from the liquid phase to the solid), evaporation or volatilization (i.e. a liquid-gas transfer), dissolution (i.e. solid-liquid transfer), and liquid-liquid transfer. It is possible that a number of these transfers occur simultaneously so that the transfer term comprises a number of different transfer processes. It is assumed here that there is no source or sink on the interphase boundary, i.e., there is no jump in the normal flux of the considered species across the boundary, so that $f_{\alpha \rightarrow \beta} = -f_{\beta \rightarrow \alpha}$.

In this instance, it is assumed that a chemical species can reach the microscopic interphase boundary by two modes of transport, namely advection and diffusion. Hence, as we have already seen from the averaging procedure in appendices 2.4.1 and 2.5, the strength of a source of a considered species in the $\alpha$-phase is given by

\[ f_{\alpha \rightarrow \beta} = \frac{1}{U_0} \int_{S_{\alpha\beta}} n^\alpha \cdot (c_\alpha (v_\alpha - w_{\alpha\beta}) + j_\alpha) dS, \]  

(2.6.22)

where $U_0$ is the volume of the REV, $S_{\alpha\beta}$ is the boundary between the $\alpha$-phase and all other phases, $n^\alpha$ is the unit outward normal vector on this surface and $w_{\alpha\beta}$ is the velocity of points on the interphase boundary. If $S_{\alpha\beta}$ is a material surface than $v_\alpha - w_{\alpha\beta} = 0$ and

\[ f_{\alpha \rightarrow \beta} = \frac{1}{U_0} \int_{S_{\alpha\beta}} n^\alpha \cdot j_\alpha dS. \]  

(2.6.23)

In this case, the chemical species crosses the interphase boundary by diffusion only. In the coffee bed model developed here non-equilibrium fluid-fluid and solid-fluid transfers will be considered. The first mechanism considered that drives transfer (in an effort to bring the system closer to equilibrium) is the difference in concentrations (or more rigorously the difference in chemical potentials) at the interface, visualised as a thin film. Therefore the rate of transfer, $f_{\alpha \rightarrow \beta}$, of the mass of the considered species, from an $\alpha$-phase to an adjacent $\beta$-phase, across an interface $S_{\alpha\beta}$ is often assumed to be proportional to the difference in concentration between the phases. Thus

\[ f_{\alpha \rightarrow \beta} = \alpha_{\alpha\beta} (c_\beta - c_\alpha). \]  

(2.6.24)
To estimate the mass transfer coefficient $\alpha_{\alpha\beta}$ the following form is used

$$j_\alpha \cdot n^\alpha = -\frac{D_\alpha (c_\beta - c_\alpha)}{\Delta_\alpha}.$$  \hspace{1cm} (2.6.25)

Here, $D_\alpha$ is the coefficient of diffusion of the considered species in the $\alpha$-phase and $\Delta_\alpha$ is the length characterising the mean size of the phase or the length over which diffusion occurs. For example, one possible definition of $\Delta_\alpha$ is $\Delta_\alpha = \frac{U_0}{S_{\alpha\beta}}$, the volume to surface ratio of the $\alpha$-phase within the REV. Then

$$f_{\alpha\rightarrow\beta} = \frac{1}{U_0} \int_{S_{\alpha\beta}} n^\alpha \cdot j_\alpha dS$$

$$= -\frac{1}{U_0} \int_{S_{\alpha\beta}} \frac{D_\alpha (c_\beta - c_\alpha)}{\Delta_\alpha} dS$$

$$= -\frac{S_{\alpha\beta}}{U_0} \left( \frac{D_\alpha (c_\beta - c_\alpha)}{\Delta_\alpha} \right)$$

$$= -\frac{S_{\alpha\beta}^*}{\Delta_\alpha} \phi_\alpha D_\alpha (c_\beta - c_\alpha),$$  \hspace{1cm} (2.6.26)

where $S_{\alpha\beta}^* = \frac{S_{\alpha\beta}}{U_0}$ is the specific surface area of the $\alpha$-phase or the surface area per unit volume. Thus it can be seen that the mass transfer coefficient is given by

$$\alpha_{\alpha\beta} = -\frac{S_{\alpha\beta}^*}{\Delta_\alpha} \phi_\alpha D_\alpha.$$  \hspace{1cm} (2.6.27)

The above derivation is for a fluid-fluid transfer. For a solid-fluid transfer a slightly different approach is used.

Under consideration here is the case where the solid matrix itself is dissolving (i.e. the soluble part of the coffee grains). It is again assumed that the porous medium is saturated and a single constituent is considered. The assumption is made that there is a thin layer of liquid next to the solid which is always saturated with the solute under consideration. This concentration is denoted by $c_{\text{sat}}$. $c_{\text{sat}}$ is the concentration in the liquid phase that would be in equilibrium with the concentration inside the solid $c_s$. This assumes that the dissolution process occurs faster than the transfer from this thin layer to the bulk of the fluid. It is now assumed that the force of extraction from this thin layer to the bulk of the fluid
is given by

\[ f_{s \rightarrow f} = \alpha_{sf} (c_{\text{sat}} - c_f). \]  

(2.6.28)

Proceeding as above it can be shown that the mass transfer coefficient from a solid phase \( s \) to a fluid phase \( f \) is given by

\[ \alpha_{sf} = \frac{S_{sf}^* \phi_s D_f}{\Delta_s}. \]  

(2.6.29)

The transfers looked at so far have been transfer of constituent or solute due to diffusion. It is also possible to have a transfer of liquid from the large pores between the grains to the small pores within the grains (or vice versa). This will occur due to a pressure imbalance between the phases due to the dissolution of the solid matrix within the grains. As was seen from the averaging procedure this term has the form

\[ \tilde{g}_{h \rightarrow l} = -\tilde{g}_{v \rightarrow h} = -\frac{\phi_v}{V_0} \int_{S_{lh}} \mathbf{n}^1 \cdot (\rho (\mathbf{v})^v (\mathbf{v})^v - \mathbf{w}_{lh}) + \langle \mathbf{i}_v \rangle^v dS. \]  

(2.6.30)

Now it is assumed that \( \langle \mathbf{i}_v \rangle^v = 0 \) and using Darcy’s Law gives

\[ \langle \mathbf{v} \rangle^v - \mathbf{w}_{lh} = -\frac{k_v (\phi_v)}{\phi_v \mu} \nabla p \]  

(2.6.31)

On \( S_{lh} \) this means that

\[ \langle \mathbf{v} \rangle^v - \mathbf{w}_{lh} = -\frac{k_v (\phi_v)}{\phi_v \mu} \frac{(p_h - p_v)}{\Delta_l}. \]  

(2.6.32)

Thus

\[ \tilde{g}_{h \rightarrow l} = -\frac{\phi_v}{V_0} \int_{S_{lh}} \mathbf{n}^1 \cdot \left( -\rho \frac{k_v (\phi_v)}{\phi_v \mu} \frac{(p_h - \hat{p}_v)}{\Delta_l} \right) dS \]

\[ = \frac{S_{lh}}{V_0} \frac{k_v (\phi_v)}{\mu} \frac{(p_h - \hat{p}_v)}{\Delta_l} \]

\[ = \phi_l S_{lh}^* \frac{k_v (\phi_v)}{\mu} \frac{(p_h - \hat{p}_v)}{\Delta_l}. \]  

(2.6.33)

Again here \( S_{lh}^* \) is the specific surface area or surface area per unit volume of the \( l \)-phase. Since there is a difference in concentration in the \( h \) and \( v \)-phases the
transfer of fluid in either direction will also result in the transfer of solute from one phase to another. This transfer will be of the following form

\[
f_{l \rightarrow h}^w = \begin{cases} 
-\varphi_l S^{*}_h \rho \frac{k_v(\varphi_v)}{\mu} \frac{\Delta l}{\Delta t} \tilde{c}_h, & \text{if } \hat{p}_h \geq \hat{p}_v \\
+\varphi_l S^{*}_h \rho \frac{k_v(\varphi_v)}{\mu} \frac{\Delta l}{\Delta t} \tilde{c}_v, & \text{if } \hat{p}_h < \hat{p}_v
\end{cases}
\] (2.6.34)

### 2.6.5 Form of individual mass transfers

It is now possible to describe the source and sink terms in the macroscopic equations arising from mass transfers in terms of the microscopic quantities of the system. Now the total mass transfer from the l-phase to the h-phase can be written as

\[
\tilde{f}_{l \rightarrow h} = \tilde{f}_{v \rightarrow h} + \tilde{f}_{s \rightarrow h} + \tilde{f}_{l \rightarrow h}^w.
\] (2.6.35)

\(\tilde{f}_{v \rightarrow h}\) represents transfer of solute between the pores within the grains and the pores between the grains due to diffusion. Now considering (2.5.31) and (2.6.24) it follows that

\[
\tilde{f}_{v \rightarrow h} = \alpha_{vh}(\tilde{c}_h - \tilde{c}_v)
= \varphi_l \varphi_v D_v S^{*}_v \frac{\Delta l}{\Delta t} (\tilde{c}_h - \tilde{c}_v)
= \varphi_l \varphi_v D_v S^{*}_v \frac{\Delta l}{\Delta t} (\tilde{c}_h - \tilde{c}_v)
= \varphi_l \varphi_v^4 D_v S^{*}_v \frac{\Delta l}{\Delta t} (\tilde{c}_h - \tilde{c}_v),
\] (2.6.36)

where \(\tau = \phi_v^{-\frac{1}{3}}\) has been used. Next transfer of solute from the solid on the surface of the grains, \(\tilde{f}_{s \rightarrow h}\) is considered. Recalling (2.5.44) and (2.6.28) and that diffusion of solute into the bulk of the fluid is the rate limiting step it follows that

\[
\tilde{f}_{s \rightarrow h} = \alpha_{sh}(c_{sat} - \tilde{c}_h)
= \varphi_l \varphi_s D_h S^{*}_h \frac{\Delta s}{\Delta s} (c_{sat} - \tilde{c}_h)
= \varphi_l (1 - \varphi_v) D_h S^{*}_h \frac{\Delta s}{\Delta s} (c_{sat} - \tilde{c}_h).
\] (2.6.37)

As outlined above the third transfer term, \(\tilde{f}_{l \rightarrow h}^w\), arises due to solute being
carried in the fluid that transfers between phases due to pressure differences between pores this is given as above by

\[
\tilde{f}_{w}^{*}_{l \rightarrow h} = \begin{cases} 
-\phi_l S_{hl}^{*} \rho k_v (\phi_v) \frac{(\tilde{p}_h - \tilde{p}_v)}{\Delta l} \tilde{c}_h, & \text{if } \tilde{p}_h \geq \tilde{p}_v \\
\phi_l S_{hl}^{*} \rho k_v (\phi_v) \frac{(\tilde{p}_h - \tilde{p}_v)}{\Delta l} \tilde{c}_v, & \text{if } \tilde{p}_h < \tilde{p}_v
\end{cases}
\]  

(2.6.38)

The macroscopic transfer term from the s-phase to the v-phase can be arrived at using (2.5.45) and (2.6.28) to get

\[
\tilde{f}_{s \rightarrow v} = \alpha_{sv} (c_{\text{sat}} - \tilde{c}_v) = \phi_l \phi_s D_v S_{sv}^{*} (c_{\text{sat}} - \tilde{c}_h).
\]  

(2.6.39)

2.6.6 Coffee bed properties

In order to proceed the quantities such as permeability, surface area, specific surface area and distances over which diffusion occurs must be expressed in terms of measurable properties of the coffee bed. We can estimate these quantities from the particle size distribution. In order to simplify things we assume that the intergranular porosity \(\phi_h\) is constant. We note that this means that the only change in porosity occurs within the l-phase. Thus it seems reasonable to assume that the pressure in the intergranular pores is always greater than or equal to the pressure in the intragranular pores, i.e. \(\tilde{p}_h \geq \tilde{p}_v\). Thus (2.6.34) simplifies to

\[
\tilde{f}_{w}^{*}_{h \rightarrow l} = (1 - \phi_h) S_{hl} \rho k_v (\phi_v) \frac{(\tilde{p}_h - \tilde{p}_v)}{\Delta l} \tilde{c}_h.
\]  

(2.6.40)

2.6.6.1 Specific surface area of l-phase

Approximating a coffee grain of diameter \(x\) by a sphere, it has a surface to volume ratio of \(\frac{6}{\pi x}\). This can be improved upon if the roundness or sphericity of the coffee grain is known. However in the absence of this we make the spherical approximation. We can use a number of equivalent spherical diameters to represent the entire size distribution. One such diameter is the diameter of the spherical particle that has the same specific surface area of that distribution. This is called the Sauter mean diameter and is defined by

\[
k_{sv} = \frac{6}{S_v},
\]  

(2.6.41)
where $S_v$ is the surface to volume ratio of the distribution which can be found from the data. The assumption $\phi_h$ is constant means that the Sauter mean diameter doesn’t change. Thus where required the specific surface area of the l-phase is given by

$$S_{hl}^* = \frac{6}{k_{sv}}.$$  \hfill (2.6.42)

In fact, we will use two separate Sauter mean diameters. In relation to flow and extraction from the surface of the grains we need to use the specific surface area of the entire distribution. We denote the corresponding Sauter mean diameter $k_{sv1}$. However, when dealing with extraction from the grain kernel, we should ignore the particles which are just broken cell fragments and don’t have a kernel of intact cells. In this case we introduce a second Sauter mean diameter $k_{sv2}$ which is representative of the specific surface area of particles above a certain diameter, chosen here to be 50 $\mu$m. This Sauter mean diameter is used for extraction from the grain kernel.

### 2.6.6.2 Specific surface area of s-phase

The specific surface area of the s-phase is more difficult to estimate. Assuming that the coffee grain is made up of solid spherical cells with the same diameter $m$ we could approximate the specific surface area by

$$S_{sv}^* = \frac{6}{m}.$$  \hfill (2.6.43)

Of course looking at the SEM images earlier this isn’t the case. Unfortunately we don’t have any information about the specific surface area of the s-phase from the grind size distribution and in practice this will form part of a lumped mass transfer coefficient which will have to be fitted to the experimental data.

### 2.6.6.3 Permeability $k_h$

The permeability can be estimated using the Kozeny-Carman equation for spheres:

$$k_h = \frac{\phi_h^3}{\kappa(1 - \phi_h)^2 S_{hl}^*}.$$  \hfill (2.6.44)
2.6 Developing macroscale equations

Here again $S_{hl}^*$ is the specific surface area, while $\kappa$ is a factor which accounts for the shape and tortuosity. Utilising the derived form for $S_{hl}^*$ gives

$$k_h = \frac{k_{v1}^2 \phi_h^3}{36\kappa(1 - \phi_h)^2} = \frac{k_{v1}^2 \phi_h^3}{36\kappa(1 - \phi_h)^2}. \quad (2.6.45)$$

The shape factor $\kappa$ is usually taken to be in the range 2–6. Experiments performed measuring the pressure drop in an airflow through compacted coffee beds estimate it at $\kappa = 3.1$.

2.6.6.4 Permeability $k_v$

Similarly, in the absence of a better description of the granular microstructure, the permeability of the grains is estimated using the Kozeny-Carman equations for the spherical cells so that

$$k_v = \frac{m^2 \phi_v^3}{180(1 - \phi_v)^2}. \quad (2.6.46)$$

In the absence of experimental data we have chosen $\kappa = 5$, which is often adopted.

2.6.6.5 Average diffusion distances

Expressions are required for $\Delta_l$ and $\Delta_s$. The distance over which diffusion from the grains to the large pores occurs, is assumed to be equal to the mean radius of the grains weighted by volume which we denote $\Delta_l = l_l$. The distance over which diffusion occurs from the surface of the solid to the h-phase is assumed to be equal to the mean radius of the coffee cells. Thus $\Delta_s = l_s$.

2.6.6.6 Coffee extraction limits

The current forms of the coffee mass transfer terms are incomplete as they do not account for the fact that for a given grind at a given temperature there is a maximum amount of coffee that can be extracted. Looking at our equations, in order to track the amount of coffee extracted we can either allow the grain porosity $\phi_v$ to change or allow the solid coffee concentration $\tilde{c}_s$ to change, or both. The decision is made here to allow $\phi_v$ to change as coffee is extracted and consider the solid concentration $\tilde{c}_s$ fixed. Thus $\phi_v$ is allowed to increase as coffee is dissolved until it reaches a point when $\phi_v$ consists of insoluble material. This maximum value
may depend on the grind size and temperature of extracting water and should be found from the experimentally determined maximum extractable solubles mass. It is also unrealistic for the mass transfer coefficients from the solid matrix surface to remain approximately constant even when there is very little soluble coffee left in the solid. This issue is sometimes solved through use of a partition coefficient. Here we make the simple assumption that the extraction term be proportional to the amount of coffee on the surface. Let \( \phi_c \) be the volume fraction of coffee in the grains. We divide this into coffee in the surface of the grains and fines \( \phi_{s,s} \), and coffee in the grain kernels \( \phi_{s,b} \), so that \( \phi_c = \phi_{s,s} + \phi_{s,b} \). Thus we can write the grain solid fraction as \( \phi_s = \phi_{s,i} + \phi_c = \phi_{s,i} + \phi_{s,s} + \phi_{s,b} \). This is illustrated in figure 2.15. The initial volume fractions of coffee in dry grains are \( \phi_{cd}, \phi_{s,sd} \) and \( \phi_{s,bd} \). Assuming that the soluble coffee is uniformly distributed within the grains the initial volume fraction everywhere is \( \phi_{cd} \). Thus at a given time the volume fractions of soluble coffee on the surface and in the grain kernels are given by

\[
\frac{\phi_{cd}}{\phi_{s,sd}} \phi_{s,s}(x, t) = \phi_{cd} \psi_s(x, t), \quad (2.6.47)
\]

\[
\frac{\phi_{cd}}{\phi_{s,bd}} \phi_{s,b}(x, t) = \phi_{cd} \psi_v(x, t), \quad (2.6.48)
\]

where \( x \) is the position within the coffee bed and \( \psi_s \) and \( \psi_v \) are the fractions of the original amount of coffee left on the grain surfaces and in the grain kernels respectively. We can now substitute \( \phi_s = \phi_{s,i} + \phi_{s,s} + \phi_{s,b} \). \( \phi_{s,i} \) represents the volume fraction of insoluble solid in the grains. Using the expressions we have developed so far this leads to two further partial differential equations for \( \psi_s \) and \( \psi_v \):

\[
\frac{\partial \psi_s}{\partial t} = -\frac{12D_h \phi_{cd}}{k_{sv1} m} \left( \frac{c_{sat} - \tilde{c}_h}{\tilde{c}_s} \right) r_s \psi_s, \quad (2.6.49)
\]

\[
\frac{\partial \psi_v}{\partial t} = -\frac{12D_v \phi_{cd}}{m^2} \left( \frac{c_{sat} - \tilde{c}_v}{\tilde{c}_s} \right) r_v \psi_v, \quad (2.6.50)
\]

where \( r_s = \frac{1}{\phi_{s,sd}} \) and \( r_v = \frac{1}{\phi_{s,bd}} \).
Figure 2.15: Location of coffee in the bed: The coffee bed consists of (intergranular) pores of volume fraction $\phi_h$ and grains of volume fraction $1 - \phi_h$. The grains consist of (intragranular) pores of volume fraction $\phi_v$ and solids of volume fraction $1 - \phi_v$. The schematic shows the breakdown of this coffee in the grains (intragranular pores are not represented for clarity). The solid consists of a soluble volume fraction $\phi_s$ and an insoluble volume fraction $\phi_{s,i}$. The soluble volume fraction is broken into a volume fraction near the surface of grains $\phi_{s,s}$ and a volume fraction in the kernels (bulk) of grains $\phi_{s,b}$.

2.6.7 Macroscale equations

Models have now been introduced for the various processes occurring in the coffee bed. The description of the process has been extended to seven coupled partial differential equations. These equations are presented in full in (2.6.51)-(2.6.57). Different presentations of the equations are possible and one equation can be reduced to an algebraic one. Boundary conditions will depend on the geometry of the problem. Initial conditions will have to be determined or inferred from experiment following the filling stage.
While these equations give estimates for the different coefficients in terms of process parameters, these parameters may not always be easy to determine accurately. Other processes which were not considered may also affect the transport of coffee and water. Thus when comparing to experiment it is necessary to introduce fitting parameters particularly to the terms controlling extraction from the grain surfaces and diffusion of coffee from the grain kernel.
2.6 Developing macroscale equations

2.6.8 Dominance of advection over mechanical dispersion and diffusion

Considering the dimensional equations (2.6.51)–(2.6.57) we can consider the relative importance of the coffee transport processes in the intergranular pores by comparing their magnitudes. This should give us an idea of the dominant transport mechanism in the bed, although of course there may be narrow regions where other balances hold. Firstly, we compare advection and dispersion. The ratio of the magnitudes of the terms is

\[ \frac{|\tilde{c}_h \tilde{v}_h|}{|D_h \nabla \tilde{c}_h|}. \] (2.6.58)

Recall that

\[ (\tilde{D}_h^i)_{ij} = \left( a_T \delta_{ij} + (a_L - a_T) \frac{v_i v_j}{|\tilde{v}_h|^2} \right) |\tilde{v}_h| = a_{ijkl} \frac{v_i v_j}{|\tilde{v}_h|}. \] (2.6.59)

We now use some characteristic scales. Note \( a_L \sim l_L \leq 500 \mu m \). Thus take \( a_{ijkl} \sim a_L, \tilde{c}_h \sim C, |\tilde{v}_h| \sim v_c, v_i \sim v_c, \) and \( z \sim L \). Thus (2.6.58) becomes

\[ \frac{Cv_c}{L} \frac{1}{l_L} \sim 10^2. \] (2.6.60)

Thus advection is approximately one hundred times larger than dispersion and so dominates. More generally advection dominates over dispersion when \( L \gg l_L \) unless there are very large concentration gradients in the bed.

The ratio of advection to diffusion is given by

\[ \frac{|\tilde{c}_h \tilde{v}_h|}{\phi^4_L D_h \nabla \tilde{c}_h}. \] (2.6.61)

Adopting similar approximations as in the dispersion case we find that

\[ \frac{Cv_c}{\phi^4_L D_h C} = \frac{Lv_c}{\phi^4_L D_h}. \] (2.6.62)

Now from the experiments, typical approximate values for these quantities are
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\( L \sim 0.05 \, \text{m}, \ v_c \sim 0.007 \, \text{m/s}, \ \phi_h \sim 0.2 \) and \( D_h \sim 2.2 \times 10^{-9} \, \text{m}^2 \, \text{s}^{-1} \). Thus

\[
\frac{Lv_c}{\phi_h^2 D_h} \sim 10^6. \tag{2.6.63}
\]

These estimates show that unless there are extremely large concentration gradients somewhere within the bed that advection dominates over diffusion.

### 2.7 Concentration of coffee in final beverage

Equations (2.6.51) tracks the concentration of coffee within the coffee bed at a given time. However, from a quality point of view, we are more interested in the concentration in the coffee pot. This is simply the mass of coffee solubles in the final beverage at a given time divided by its volume. Suppose the coffee solution exits the bed through a surface \( S_f \) and the normal fluid velocity on this surface (in the Darcy sense) through a surface element \( dS \), at position \( x \), is given by \( u(x, t) \). Then the coffee mass that has exited the bed at a given time \( T \) is

\[
\int_0^T \int_{S_f} u(x, t) c_h(x, t) dS \, dt. \tag{2.7.1}
\]

Similarly the volume at a given time \( T \) is

\[
\int_0^T \int_{S_f} u(x, t) dS \, dt, \tag{2.7.2}
\]

and so the concentration in the pot \( c_p(T) \) is

\[
c_p(T) = \frac{\int_0^T \int_{S_f} u(x, t) c_h(x, t) dS \, dt}{\int_0^T \int_{S_f} u(x, t) dS \, dt}. \tag{2.7.3}
\]

The extraction yield is simply got by dividing the mass of coffee solubles in the pot at a given time by the mass of the initial dry coffee bed.

### 2.8 Numerical simulations

Numerical simulations of the experiments in sections 2.2.3 and 2.2.4 are conducted using the model equations. The equations can be reduced in both of these cases.
2.8 Numerical simulations

2.8.1 Batch-wise brewing

In the French press type brewing apparatus there is no pressure induced flow and we assume the solution in the h-phase is well mixed, since only the average concentration in this phase is measured anyway. Thus all spatial derivatives in the equations drop out leaving a system of ordinary differential equations. In order to solve the system we require some initial conditions. Here we need to make some assumptions, since we do not model the initial infiltration of the water into the grains when the coffee and water are mixed. Firstly, we assume that the grains are saturated with water initially. We further assume that the initial concentration in the h-phase is zero, so that none of the coffee has dissolved from the surface of the grains. It is also necessary to give an initial condition for the concentration in the v-phase. It is assumed initially that all the soluble coffee in the grains has dissolved into the v-phase. This is of course unlikely to be the case. However, since coffee diffusion from the v-phase to the h-phase is thought to be the rate limiting process, occurring much slower than dissolution of coffee, this assumption is unlikely to have much impact on the simulation results. We also assume that, only a change in porosity in the intact cells in the grain kernel will result in a change in pressure in the v-phase, since any pressure imbalance in the damaged cells on the grain surface would be almost instantaneously corrected. Thus, as all coffee in kernel is assumed dissolved initially, no pressure difference between phases will occur. Note the value of intragranular porosity $\phi_v = 0.56$ is adopted here for dry coffee in air. Allowing for these assumptions the following system of equations are solved numerically in MATLAB®:

\[
\begin{align*}
\phi_h \frac{d\tilde{c}_h}{dt} &= -\alpha^* (1 - \phi_h) \phi_v^4 D_v \frac{6}{k_{sv2l_1}} (\tilde{c}_h - \tilde{c}_v) \\
&\quad + \beta^* (1 - \phi_h) \frac{12D_h \phi_{cd}}{k_{sv1m}} (c_{sat} - \tilde{c}_h) \psi_s, \quad (2.8.1) \\
\frac{d}{dt}(\phi_v \tilde{c}_v) &= -\alpha^* \phi_v^4 D_v \frac{6}{k_{sv2l_1}} (\tilde{c}_h - \tilde{c}_v), \quad (2.8.2) \\
\frac{d\phi_v}{dt} &= -\frac{1}{r_s} \frac{\partial \psi_s}{\partial t}, \quad (2.8.3) \\
\frac{d\psi_s}{dt} &= -\beta^* \frac{12D_h \phi_{cd}}{k_{sv1m}} \left( \frac{c_{sat} - \tilde{c}_h}{\tilde{c}_s} \right) r_s \psi_s, \quad (2.8.4)
\end{align*}
\]

with initial conditions
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\[
\begin{align*}
\tilde{c}_h(0) &= 0, & \tilde{c}_v(0) &= c_{v0}, & \phi_v(0) &= \phi_{v0}, & \psi_s(0) &= 1. 
\end{align*}
\] (2.8.5)

The parameters \( \alpha^* \) and \( \beta^* \) are used as fitting parameters to fit the experimental results. The mass transfer coefficients depend on the volume fraction of the interstitial water in the coffee bed in question, so the fitting parameters are just intended to correct for errors in the other parameters in the mass transfer coefficient. Thus we look for values of \( \alpha^* \) and \( \beta^* \) which fit both experiments equally well. The initial volume fractions of coffee \( \phi_{s,sd} \) and \( \phi_{s,bd} \) can, to some extent, be estimated from the grind size distribution but here we will use them to allow for any differences between the batch extraction and coffee flow-through-cell experiments. These differences may arise, for example, due to the fact that we do not model the initial water infiltration into the coffee grains. The parameters used in the simulations are listed in table 2.1. The other parameters are all measured experimentally, estimated from experiments or sourced in the literature. The value for the coffee solubility, \( c_{\text{sat}} \), is estimated from the highest observed concentration across the four experiments. The diffusion coefficient is for caffeine in water at 80°C [37]. This would be slightly higher at 90°C. However this is only an estimate of the effective diffusion coefficient of coffee in water. The fitting parameters are used to correct any errors in these parameters. The comparison between the numerical solution and the experimental results is shown in figure 2.16.

\[\text{(a)}\]  
\[\text{(b)}\]

**Figure 2.16:** Comparison between numerical solution (\( \cdots \)) with parameters from table 2.1 and experiment (*) for the batch extraction experiments for (a) JK drip filter grind and (b) Cimbali #20 grind.
2.8 Numerical simulations

Parameter | JK Drip filter | Cimbali #20 |
---|---|---|
φ_v0 | 0.6444 | 0.6120 |
φ_h | 0.8272 | 0.8272 |
k_{sv1} | 27.35μm | 38.77μm |
k_{sv2} | 322.49μm | 569.45μm |
l_t | 282μm | 463μm |
D_h = D_v | 2.2 × 10^{-9} m^2 s^{-1} | 2.2 × 10^{-9} m^2 s^{-1} |
ρ | 965.3 kg m^{-3} | 965.3 kg m^{-3} |
μ | 0.315 × 10^{-3} Pa s | 0.315 × 10^{-3} Pa s |
m | 30μm | 30μm |
c_{sat} | 212.4 kg m^{-3} | 212.4 kg m^{-3} |
c_s | 1400 kg m^{-3} | 1400 kg m^{-3} |
κ | 3.1 | 3.1 |
φ_{cd} | 0.143435 | 0.122 |
φ_{s, sd} | 0.059 | 0.07 |
φ_{s, bd} | 0.084435 | 0.052 |
α* | 0.1833 | 0.0881 |
β* | 0.0447 | 0.0086 |
r_s | 16.94 | 14.28 |
c_v0 | 183.43 kg m^{-3} | 118.95 kg m^{-3} |

Table 2.1: Parameters for simulation of the batch extraction experiments.

2.8.2 Cylindrical brewing chamber

The cylindrical brewing chamber geometry also allows us to make some simplifications to the general model. Assuming that the coffee bed properties are homogeneous in any cross section, the equations can be reduced to one spatial dimension, parallel to the flow direction. Thus the bed depth is labelled by the z-coordinate. The height of the coffee bed is L with the bottom (filter exit) at z = 0 and the top (filter entrance) at z = L. For the experiments here it is shown in section 2.6.8 that advection dominates over diffusion and mechanical dispersion, so these two processes are neglected. This means we just require one concentration boundary condition for ˜c_h. We use the condition that the water entering at the top z = L has zero concentration. The pressure boundary conditions are ˜p_h = Δp at z = L and ˜p_h = 0 at z = 0. Δp is the pressure difference across the bed. In these experiments there is a large pressure difference across the bed which can lead to bed compaction and a reduction in the porosity. Thus the porosity cannot be measured a priori. It is assumed that φ_h adjusts to the pressure while φ_v stays constant. We then choose φ_h by matching the volume flow
from Darcy’s Law and the Kozeny-Carman equation to the experimental volume flow. Once again the initial conditions need to be inferred. It is assumed that once brewed coffee starts to flow from the bed that the bed is fully saturated with liquid. Again it is assumed that all the coffee in the grain kernels has dissolved into the intragranular pores (v-phase) during filling and this is uniformly distributed in the bed. It is also necessary to estimate the initial concentration \( \tilde{c}_h \) as a function of \( z \). Based on the initial exiting concentrations we assume for the fine grind (JK) that initially \( \tilde{c}_h \) is at the coffee solubility throughout the h-phase. For the coarser grain, (Cimbali # 20), we assume a linear concentration profile in the h-phase, rising from zero at the top to the initial exiting concentration at the bottom of the bed. Thus it is assumed that some extraction from the fines and broken surface cells occurs during filling. To this end the amount of surface coffee is uniformly reduced by the corresponding amount of coffee initially present in the h-phase. In reality we would expect more extraction would have occurred at the top of the bed during filling than the bottom, but, in the absence of experimental guidance, we make the simplest assumption. As with the batch experiments the assumptions mean that \( \tilde{p}_h = \tilde{p}_v \). Based on these assumptions the reduced set of equations to model extraction in the cylindrical brewing chamber is given by

\[
\phi_h \frac{\partial \tilde{c}_h}{\partial t} = \frac{k_{sv}^2 \phi_h^3}{36 \kappa \mu (1 - \phi_h)^2} \frac{\partial}{\partial z} \left( \tilde{c}_h \left( \frac{\partial \tilde{p}_h}{\partial z} + \rho g \right) \right) - \alpha^* (1 - \phi_h) \phi^4 \frac{4}{D_v} k_{sv}^2 l_t (\tilde{c}_h - \tilde{c}_v) + \beta^* (1 - \phi_h) \frac{12 D_h \phi_{cd}}{k_{sv} m} (c_{sat} - \tilde{c}_h) \psi_s,
\]

(2.8.6)

\[
\frac{\partial^2 \tilde{p}_h}{\partial z^2} = 0,
\]

(2.8.7)

\[
\frac{\partial}{\partial t} (\phi_v \tilde{c}_v) = -\alpha^* \phi^4 \frac{4}{D_v} D_v \frac{6}{k_{sv}^2 l_t} (\tilde{c}_h - \tilde{c}_v),
\]

(2.8.8)

\[
\frac{\partial \phi_v}{\partial t} = \frac{1}{r_s} \frac{\partial \psi_s}{\partial t},
\]

(2.8.9)

\[
\frac{\partial \psi_s}{\partial t} = -\beta^* \frac{12 D_h \phi_{cd}}{k_{sv} m} \left( \frac{c_{sat} - \tilde{c}_h}{\tilde{c}_s} \right) r_s \psi_s,
\]

(2.8.10)

for
with initial conditions

\[
\begin{align*}
\tilde{c}_h(z,0) &= c_{h0}(z), & \tilde{c}_v(z,0) &= c_{v0}, \\
\phi_v(z,0) &= \phi_{v0}, & \psi_s(z,0) &= \psi_{s0}, \\
\end{align*}
\]

and boundary conditions

\[
\begin{align*}
\tilde{c}_h(L,t) &= 0, & \tilde{p}_h(0,t) &= 0, & \tilde{p}_h(L,t) &= \Delta p.
\end{align*}
\]

The initial concentration profile in the JK drip filter grind is given by \(c_{h0}(z) = c_{\text{sat}}\). In the Cimbali #20 grind the initial concentration is given by \(c_{h0}(z) = \frac{c_{\text{max}}}{L}(L - z)\). Some of the parameters are the same as those in the batch extraction case. Any new parameters or parameters that have changed are included in table 2.2. The numerical solution is found using finite differences in the spatial direction and the method of lines. It should be noted that any initial discontinuities in the initial and boundary conditions will be smoothed out by numerical diffusion. If accuracy is required in the initial stages a large number of steps should be used in the spatial partition, or a more sophisticated numerical scheme implemented. The comparison between the numerical solution and the experimental results is shown in figure 2.17.

\section{Conclusion}

The coffee extraction process can be described very effectively using mathematical models. In this chapter a general model is introduced to describe coffee extraction by hot water from a bed of coffee grains. The coffee bed is modelled as a saturated porous medium using a double porosity model. The bed consists of two kinds of pores: pores between the grains (intergranular) and pores within the grains (intragranular). Flow of liquid within the coffee bed is modelled using Darcy’s Law and the Kozeny-Carman equation. Motivated by experiment, extraction of
2. MATHEMATICAL MODELLING OF THE COFFEE BREWING PROCESS

<table>
<thead>
<tr>
<th>Parameter</th>
<th>JK Drip filter</th>
<th>Cimbali #20</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi_{v0}$</td>
<td>0.6231</td>
<td>0.6218</td>
</tr>
<tr>
<td>$\phi_h$</td>
<td>0.2</td>
<td>0.25</td>
</tr>
<tr>
<td>$c_{\text{max}}$</td>
<td>—</td>
<td>82.63 kg m$^{-3}$</td>
</tr>
<tr>
<td>$c_s$</td>
<td>1400 kg m$^{-3}$</td>
<td>1400 kg m$^{-3}$</td>
</tr>
<tr>
<td>$\phi_{s,sd}$</td>
<td>0.11</td>
<td>0.07</td>
</tr>
<tr>
<td>$\phi_{s,hd}$</td>
<td>0.033435</td>
<td>0.052</td>
</tr>
<tr>
<td>$\alpha^*$</td>
<td>0.1833</td>
<td>0.0881</td>
</tr>
<tr>
<td>$\beta^*$</td>
<td>0.0447</td>
<td>0.0086</td>
</tr>
<tr>
<td>$r_s$</td>
<td>9.09</td>
<td>14.28</td>
</tr>
<tr>
<td>$c_{e0}$</td>
<td>78.88 kg m$^{-3}$</td>
<td>118.95 kg m$^{-3}$</td>
</tr>
<tr>
<td>$\Delta p$</td>
<td>230 000 Pa</td>
<td>65 000 Pa</td>
</tr>
<tr>
<td>$L$</td>
<td>0.0405 m</td>
<td>0.0526 m</td>
</tr>
</tbody>
</table>

**Table 2.2**: Parameters for simulation of the cylindrical brewing chamber extraction experiments.

**Figure 2.17**: Comparison between numerical solution (–) with parameters from table 2.2 and experiment (*) for the cylindrical brewing chamber extraction experiments for (a) JK drip filter grind and (b) Cimbali #20 grind.

Coffee from the coffee grains is modelled using two mechanisms. Coffee on the damaged grain surfaces and in coffee cell fragments or fines extracts quickly into the intergranular pores due to a relatively low mass transfer resistance. Coffee in intact cells in the grain kernels, first extracts into the intragranular pores and then slowly diffuses through the grain into the intergranular pores.

The model is parametrised using experimental data. Numerical simulations are performed and fitted to data. It is shown that the developed models can quantitatively describe extraction from ground coffee in two situations: in a well
stirred dilute suspension of coffee grains, and in a packed coffee bed. The extraction curves fit the data for both a fine and a coarse grind, as the parameters in the model vary with the surface area and the mean grain radius of the grind size distribution. Provided the grind size distribution is known, and the physics of extraction is the same, the model should work well for an even wider range of grind sizes.

There is a wide variety of topics in the area of coffee extraction and coffee brewing in general which may benefit from further mathematical modelling and investigation. The model described can be easily generalised to describe standard coffee brewing techniques. It can also be extended to include unsaturated flow during water infiltration into the coffee bed and drainage of water from the coffee bed. Some preliminary work on this is presented in chapter 5. The model can also easily be extended to model the extraction of a number of different coffee constituents rather than just a single entity. This may be useful if the influence on flavour of particular constituents (or groups of constituents which extract at similar rates) can be identified. The model is also adaptable to different bed geometries.

In terms of modelling drip filter brewing, the assumption of a static bed may need to be relaxed, particularly in order to model extractions where the extracting fluid is delivered via a single jet, rather than dispersed by a shower-head. In the case of a single jet the coffee bed experiences significant mixing with the final bed shape revealing a central cavity such as that shown in figure 2.18. Such mixing where coffee grains are entrained in the flow in the filter is likely to lead to a faster extraction in these grains. The extraction in the bed would also tend to be less uniform than a shower head. However in the case of grinds commonly used in drip filter brewing apparatus, use of a single jet is found to deliver better coffee, with coffee from a shower head tending to be over-extracted. This is likely due to the single jet punching a hole in the bed and reducing the overall bed resistance and thus the residence time. For coarse grinds dosing with a shower head is found to be better, leading to a more uniform extraction. To investigate
the effect of mixing, the models here could be extended to two-phase flow by relaxing the static assumption. Alternatively the models of extraction kinetics could be applied to a single grain and incorporated in a discrete element method (DEM) or computational fluid dynamics/discrete element method (CFD-DEM) simulation. The model is presented for isothermal conditions but may also be extended to include heat transfers within the coffee bed. In this case the influence of temperature on extraction must be determined and incorporated.
CHAPTER 3

COFFEE EXTRACTION IN A WELL MIXED SYSTEM

3.1 Introduction

In chapter 2, a general double porosity model of coffee extraction in a fixed coffee bed was presented. Making certain assumptions, it was shown that the model could reproduce experimentally measured extraction curves from batch-wise coffee extractions in a fixed water volume. This experiment was described in section 2.2.3. By applying model reduction to the general equations we can specialise them to describe this situation. This was done on a somewhat ad-hoc basis in section 2.8.1 and numerical solutions were generated. In this chapter we will consider the model reduction and solution in the case of the batch-wise coffee extraction in more detail. We will consider the system as being well-mixed so that all spatial derivatives will be removed from the equations and leave a system of ordinary differential equations. Analysing extraction from a well-mixed, dilute suspension of coffee grains is of interest, as it allows us to investigate the extraction kinetics from the coffee grains, independent of the complications introduced by the advection and mechanical dispersion occurring in pressurised flow through a tortuous packed coffee bed. The general model from chapter 2 will be specialised to describe extraction from a dilute suspension of coffee grains. The dominant mechanisms during the extraction are then identified by non-dimensionalising the
equations. Approximate solutions are formed based on the dominant processes during different stages of the extraction. The approximate solutions are compared with numerical solutions of the system and also with experimental data presented in section 2.2.3. The work in this chapter is published in ref. [49].

### 3.1.1 General coffee extraction model

We begin here with the general coffee extraction model comprising equations (2.6.51)–(2.6.57). This system of equations includes a term for transfer of fluid (and coffee solubles as a result) between the h-phase and v-phase due to differences in pressures. This correction is difficult to model accurately without further experimental insight and is thought to occur much faster than other bed processes. Also as discussed in section 2.6 this term is dependent on the description of the influence of solute concentration on the coffee solution density. Neglecting the term here means we assume that solid coffee and water occupy the same space as that coffee dissolved in the water. As coffee diffuses out of the grain the water needed to replace that coffee is not accounted for in the model. For these reasons the coffee solution transfer terms are neglected in the presentation of the equations here. The equations are:

\[
\phi_h \frac{\partial c^*_h}{\partial t^*} = \frac{k^2}{36 \kappa \mu (1 - \phi_h)^2} \nabla^* \cdot \left( c^*_h (\nabla^* p^*_h + \rho g) \right) + \phi_h D_h \nabla^{*2} c^*_h \\
+ \phi_h D^b \cdot \nabla^{*2} c^*_h - (1 - \phi_h) \phi_v \frac{4}{3} D_v \frac{6}{k_{sv2l}} (c^*_h - c^*_v) \\
+ (1 - \phi_h) \frac{12 D_{hv} \phi_{cd}}{k_{sv1m}} (c_{sat} - c^*_h) \psi^*_s, \\
\\text{(3.1.1)}
\]

\[
\nabla^{*2} p^*_h = 0, \quad \text{(3.1.2)}
\]

\[
\frac{\partial}{\partial t^*} (\phi_v c^*_v) = \phi_v \frac{4}{3} D_v \frac{6}{k_{sv2l}} (c^*_h - c^*_v) + \frac{12 \phi_{cd} D_v}{m^2} (c_{sat} - c^*_v) \psi^*_v, \quad \text{(3.1.3)}
\]

\[
\frac{\partial \phi^*_v}{\partial t^*} = - \frac{1}{r_s \partial t^*} - \frac{1}{r_v \partial t^*}, \quad \text{(3.1.4)}
\]

\[
\frac{\partial \psi^*_s}{\partial t^*} = - \frac{12 D_{hv} \phi_{cd}}{k_{sv1m}} \left( \frac{c_{sat} - c^*_h}{c_s} \right) r_s \psi^*_s, \quad \text{(3.1.5)}
\]

\[
\frac{\partial \psi^*_v}{\partial t^*} = - \frac{12 D_v \phi_{cd}}{m^2} \left( \frac{c_{sat} - c^*_v}{c_s} \right) r_v \psi^*_v. \quad \text{(3.1.6)}
\]

In contrast to chapter 2, variables in the dimensional model which will appear in scaled form in the dimensionless model are denoted by an asterisk. Note that
3.2 Model specialisation

this includes some intrinsically dimensionless variables which are normalised in the dimensionless model. In the following sections this model will be specialised to model the experimental results for extraction of coffee from a dilute suspension of coffee grains.

3.2 Model specialisation

The experiments described in section 2.2.3 involves mixing 60 g of coffee grind with 0.5 L of hot water and measuring the concentration of the extracted species as a function of time. In this situation the coffee extraction model can be simplified. Firstly it is assumed that the solution in the liquid outside the grains (h-phase) is well mixed, since only the average is measured anyway. As a result, the solution in the h-phase has uniform concentration. This means that the spatial derivatives in the model disappear and we have the following system of ordinary differential equations:

\[
\begin{align*}
\phi_h \frac{dc^*_h}{dt^*} &= -\alpha^*(1 - \phi_h)\phi_v^* \frac{4}{k_{sv}l} (c^*_h - c^*_v) \\
&\quad + \beta^*(1 - \phi_h) \frac{12D_h}{k_{sv}m} (c_{sat} - c^*_h) \psi^*_s, \\
\frac{dc^*_v}{dt^*} &= \alpha^* \phi_v^* \frac{1}{k_{sv}l} (c^*_h - c^*_v) + \gamma^* \phi_v^* - \frac{12D_v}{m^2} (c_{sat} - c^*_v) \psi^*_v \\
&\quad - c^*_v \frac{d\phi_v^*}{dt^*}, \\
\frac{d\phi_v^*}{dt^*} &= -\frac{1}{r_s} \frac{d\psi^*_s}{dt^*} - \frac{1}{r_v} \frac{d\psi^*_v}{dt^*}, \\
\frac{d\psi^*_s}{dt^*} &= -\beta^* \frac{12D_h}{k_{sv}m} \left( \frac{c_{sat} - c^*_h}{c_s} \right) r_s \psi^*_s, \\
\frac{d\psi^*_v}{dt^*} &= -\gamma^* \frac{12D_v}{m^2} \left( \frac{c_{sat} - c^*_v}{c_s} \right) r_v \psi^*_v.
\end{align*}
\]

\( t^* > 0, \quad (3.2.6) \)

\( c^*_h(0) = c^*_{h0}, \quad c^*_v(0) = c^*_{v0}, \quad \phi^*_v(0) = \phi^*_{v0}, \quad \psi^*_s(0) = \psi^*_{s0}, \quad \psi^*_v(0) = \psi^*_{v0}. \quad (3.2.7) \)

The last term now appearing on the right hand side of equation (3.2.2) is a volume correction term to allow for changes in the intragranular porosity. Additional
parameters $\alpha^*$, $\beta^*$ and $\gamma^*$ are introduced here to fit the model to experiment. These parameters are necessary due to the difficulty in obtaining accurate values for some of the model parameters. For example the diffusion coefficient used for coffee solubles will be for that of caffeine in water. However caffeine diffusivity may differ from the average coffee diffusivity in water and the extraction of many coffee components from a grain’s cellular matrix is hindered to a greater degree than that of caffeine [37]. Parameters relating to coffee grain properties, such as the cell radius and external and particularly internal specific surface areas are similarly difficult to measure. Thus fitting parameters are required. Clearly to solve this system we need to prescribe initial conditions for each of the dependent variables. This model does not include the addition of the water to the dry coffee grains or the infiltration of water into the intragranular pores. Rather it is assumed that this infiltration occurs quickly and the model starts with the grains saturated with water. This raises the question as to what initial conditions we should use for the model. How much of the coffee has dissolved during the addition of water to the coffee and the infiltration of water into the coffee grains?

In the absence of experimental data or separate modelling of this initial filling stage we will need to prescribe appropriate initial conditions. The simplest choice would be to assume that no coffee dissolves during this filling stage, so that all initial concentrations are zero, but this may not be the most useful.

To reduce the steps we have to take when non-dimensionalising the problem it is useful to make some simplifying steps at this stage based on our knowledge of the process. First of all the sum of the intragranular pore volume fraction, and the soluble coffee volume fraction is conserved. This is described by equation (3.2.3). Integrating this equation with respect to time we obtain

$$\phi_v^*(t) + \frac{1}{r_s} \psi_s^*(t) + \frac{1}{r_v} \psi_v^*(t) = K,$$

with $K$ a constant. We can determine this constant by denoting the final intragranular porosity when all soluble coffee has been dissolved as $\phi_v^\infty$. The value of $\phi_v^\infty$ can be estimated from data on the percentage of soluble coffee for a particular coffee grind. Thus we have

$$\phi_v^*(t) = \phi_v^\infty - \frac{1}{r_s} \psi_s^*(t) - \frac{1}{r_v} \psi_v^*(t).$$
Using this equation and (3.2.3) we can eliminate $\phi^*_v$ from the model system of equations. We can further simplify the system by noting that the change in intragranular porosity during extraction is small relative to the final (or initial) value of intragranular porosity. More explicitly $\phi_{s, sd} + \phi_{s, bd} = r_s^{-1} + r_v^{-1} \ll \phi^\infty_v$. Thus we make the approximation that $\phi^*_v \approx \phi^\infty_v$ in the equations. Initial conditions should be adjusted to account for this. Also the volume correction term now drops out of equation (3.2.2).

Finally we consider the fitting parameters $\alpha^*$, $\beta^*$ and $\gamma^*$. Experimental data for $c^*_v$ presented in section 2.2.3 reveals a rapid initial extraction followed by a much slower extraction. We can use this data to fit $\alpha^*$ and $\beta^*$. As dissolution of coffee within the grains and diffusion of coffee from the grains occur consecutively, fitting the parameter $\alpha^*$ rather than $\gamma^*$ corresponds to the assumption that diffusion of coffee from the grains is the rate controlling step in this series. The fitting parameter $\gamma^*$ for the rate of dissolution of coffee from the cell walls within the grains cannot be determined independently from $\alpha^*$ from experimental data available in section 2.2.3. This is because the intragranular concentration $c^*_v$ is not measured experimentally. A reasonable guess however may be that it has a value similar to the surface dissolution fitting parameter $\beta^*$. In reality, due to a larger surface area per unit volume within the coffee grains, it is likely $\gamma^* > \beta^*$. The timescale on which surface dissolution occurs is much shorter than that of diffusion of coffee from the grain kernels. Also based on the assumption $\gamma^* > \beta^*$, dissolution from cell walls within the grains occurs on a similar timescale to surface dissolution. Thus diffusion through grain cellular structure is the rate controlling step in the extraction of solubles from the intact cells in the grain kernels. This suggests that we can approximate these processes by assuming that all the coffee in the grain kernels dissolves very quickly initially into the intragranular pores and extraction is just controlled from there. This of course means that the concentration in the intragranular pores and the intragranular porosity will be incorrect at least for a short period initially but in any case we have no data for comparison. The approximation has the advantage of giving us easy to calculate initial conditions. To ensure conservation of coffee during extraction we need to be careful when prescribing initial conditions. Finally we assume that initially none of the coffee on the grain surfaces has dissolved. Based on this discussion we choose the following dimensional initial conditions:
3. COFFEE EXTRACTION IN A WELL MIXED SYSTEM

\[ c_h^*(0) = 0, \quad c_v^*(0) = \frac{\phi_{s,bd}}{\phi_\infty c_s}, \]  
(3.2.10)
\[ \psi_s^*(0) = 1, \quad \psi_v^*(0) = 0. \]  
(3.2.11)

Since \( \psi_v^*(0) = 0 \), we have reduced the system to the following three ordinary differential equations:

\[ \frac{dc_h^*}{dt^*} = -\alpha \frac{1 - \phi_h}{\phi_h} \phi_v^* \frac{4}{3} D_v \frac{6}{k_{sv2} l} (c_h^* - c_v^*) \]
\[ + \beta \frac{1 - \phi_h}{\phi_h} 12 D_h \phi_{cd} (c_{sat} - c_h^*) \psi_s^*, \]  
(3.2.12)
\[ \frac{dc_v^*}{dt^*} = \alpha \phi_v^* \frac{4}{3} D_v \frac{6}{k_{sv2} l} (c_h^* - c_v^*), \]  
(3.2.13)
\[ \frac{d\psi_s^*}{dt^*} = -\beta 12 D_h \phi_{cd} \frac{c_{sat} - c_h^*}{c_s} \frac{r_s}{c_s} \psi_s^*, \]  
(3.2.14)

3.3 Non-dimensionalisation

There are three main timescales evident in the equations: The timescale on which the coffee dissolves within the grains, the timescale on which coffee dissolves from the grain surfaces and finally the timescale on which coffee diffuses from the intragranular pores to the surrounding fluid. We have already made the assumption that the diffusion of coffee from the intragranular pores occurs on a much longer timescale than dissolution of coffee within the grains. On the basis that these processes occur consecutively, only diffusion of coffee from the intragranular pores is considered as the rate limiting step. Thus there are two remaining timescales to consider. We denote the bulk diffusion timescale by \( t_d \) and the surface dissolution timescale by \( t_s \). For the fine grind parameters in ref. [51] the values of the timescales are \( t_s = 1.184 \text{ s} \) and \( t_d = 42.231 \text{ s} \). For the coarse grind parameters the values of the timescales are \( t_s = 19.389 \text{ s} \) and \( t_d = 270.493 \text{ s} \).

To begin we scale the equations on the slow timescale. We will presently see that the problem is of a boundary layer type, and using the diffusion timescale is equivalent to an outer scaling. The concentration scale for the fluid surrounding the grains is chosen by balancing the increase in concentration per unit time with the transport of coffee solubles from the kernels of the grain by diffusion. The concentration scale in the intragranular pores is chosen to be equal to the
coffee solubility in water $c_{\text{sat}}$. The scale for $\psi_s^*$ can be chosen either from the initial condition $\psi_s^*(0) = \psi_{s0}^* = 1$ or by balancing the source term for the transfer of coffee from the grain surfaces with the other two terms in equation (3.2.12). Either of these scales allow us to solve the problem so we adopt the former which is more tractable. Thus the scales are

$$c^*_h \sim c_{\text{sat}} \phi_v^\infty (1 - \phi_h), \quad c^*_v \sim c_{\text{sat}}, \quad (3.3.1)$$

$$t^* \sim t_d = \frac{k_{sv2l}}{6\alpha^* \phi_v^\infty \frac{1}{2} D_v}, \quad \psi_s^* \sim \psi_{s0}^* = 1. \quad (3.3.2)$$

Before the dimensionless equations are presented we tidy up the presentation by introducing some dimensionless parameters. First the ratio of the surface dissolution timescale to the timescale of diffusion of coffee from the grain kernels is denoted by

$$\epsilon = \frac{\alpha^* D_v k_{sv1} m \phi_v^\infty \frac{1}{2} c_s}{2 \beta^* D_h k_{sv2l} \phi_{cd} c_{\text{sat}} r_s}. \quad (3.3.3)$$

Also we introduce

$$b_1 = \frac{2 \beta^* D_h k_{sv2l} \phi_{cd} \phi_v^\infty \frac{1}{2} (1 - \phi_h) c_{\text{sat}} r_s}{\alpha^* D_v k_{sv1} m \phi_h c_s}, \quad b_2 = \frac{2 \beta^* D_h k_{sv2l} \phi_{cd} (1 - \phi_h)}{\alpha^* D_v k_{sv1} m \phi_h \phi_v^\infty \frac{1}{4}}. \quad (3.3.4)$$

For parameters of both fine and coarse grinds the parameter $\epsilon \ll 1$, while $b_1$ and $b_2$ are both $O(1)$. We represent the non-dimensional initial concentration of coffee in the intragranular pores by the parameter $\gamma_1$. Thus our equations and initial conditions on the diffusion timescale are

$$\epsilon \frac{dC_h}{d\tau} = -eb_2 C_h \Psi_s + \frac{b_2}{b_1} \Psi_s - \epsilon^2 b_1 C_h + \epsilon C_v, \quad (3.3.5)$$

$$\frac{dC_v}{d\tau} = eb_1 C_h - C_v, \quad (3.3.6)$$

$$\epsilon \frac{d\Psi_s}{d\tau} = eb_1 C_h \Psi_s - \Psi_s, \quad (3.3.7)$$

$$C_h(0) = 0, \quad C_v(0) = \gamma_1, \quad \Psi_s(0) = 1. \quad (3.3.8)$$

On the long timescale, this suggests that at leading order $\Psi_s$ relaxes to a steady state zero value, while $C_v$ decays exponentially with time. It is clear from the form of the equations that we have a singular perturbation and so initial
conditions may not be applied to the outer solutions. For this system we have a number of ways to solve the problem. To begin with we consider the solution of the problem in a phase plane.

### 3.4 Model analysis and asymptotic solutions

#### 3.4.1 Phase plane analysis

In the case of extraction of coffee from a suspension of coffee grains, unlike the system for extraction from a packed coffee bed, we have conservation of coffee in the system. Thus we can reduce the number of equations in the system by one by using this property. We note that

\[
\frac{dC_h}{d\tau} + \frac{dC_v}{d\tau} + \frac{b_2}{b_1} \frac{d\Psi_s}{d\tau} = 0, \tag{3.4.1}
\]

and integrating with respect to \(\tau\) gives

\[
C_h(\tau) + C_v(\tau) + \frac{b_2}{b_1} \Psi_s(\tau) = C, \tag{3.4.2}
\]

with \(C\) constant. Using the initial conditions we can write

\[
\Psi_s(\tau) = 1 - \frac{b_1}{b_2} \left( C_h(\tau) + C_v(\tau) - \gamma_1 \right). \tag{3.4.3}
\]

Thus \(\Psi_s\) can be eliminated from the system to give

\[
\epsilon \frac{dC_h}{d\tau} = \left( \frac{b_2}{b_1} - \epsilon b_2 C_h \right) \left( 1 - \frac{b_1}{b_2} (C_h + C_v - \gamma_1) \right) - \epsilon^2 b_1 C_h + \epsilon C_v, \tag{3.4.4}
\]

\[
\frac{dC_v}{d\tau} = \epsilon b_1 C_h - C_v, \tag{3.4.5}
\]

with initial conditions given by (3.3.8). Writing the equations in this form has some advantages. The number of equations is reduced to two, which facilitates the investigation of the solutions for \(C_h\) and \(C_v\) on a phase plane. We find the nullclines by setting the right hand sides of equations (3.4.4) and (3.4.5) equal to zero. The physically relevant region of interest in the problem is \(C_h > 0, C_v > 0\) and \(C_h + C_v < \frac{b_2}{b_1} + \gamma_1\). Once the nullclines are drawn on the phase plane it is relatively straightforward to plot the solution on the plane. The phase planes
and solution trajectories for the fine and coarse grind experiments are shown in figure 3.1. In both cases, we see a rapid transition from the initial point to the $C_h$ nullcline before a much slower transition along the slow manifold towards a stable equilibrium point at the intersection of the nullclines. This stable equilibrium is given by

$$C_h = \frac{b_1 \gamma_1 + b_2}{b_1 (b_1 \epsilon + 1)}, \quad C_v = \frac{\epsilon (b_1 \gamma_1 + b_2)}{b_1 \epsilon + 1}. \quad (3.4.6)$$

---

**Figure 3.1:** Phase plane solutions: The phase plane diagrams are given for (a) fine grind parameters $\epsilon = 0.028$, $b_1 = 5.239$, $b_2 = 2.897$ and $\gamma_1 = 0.70$ (JK drip filter grind) and (b) coarse grind parameters $\epsilon = 0.071$, $b_1 = 1.99$, $b_2 = 1.35$ and $\gamma_1 = 0.5$ (Cimbali #20 grind). Solution trajectories and direction fields are plotted in both cases. The magnitude of the direction field is represented by the size of the blue direction vectors.

It is clearly useful to be able to reduce the number of equations to two, but it is more difficult to understand the physical meaning of the individual terms when the equation is written in this form. Thus when proceeding with the determination of approximate solutions of the problem the system of three differential equations will be used.
3. COFFEE EXTRACTION IN A WELL MIXED SYSTEM

3.4.2 Perturbation solutions on the bulk diffusion (outer) timescale

We use the following expansions for the bulk diffusion timescale

\[ C_h \sim C_{h0} + \epsilon C_{h1} + \epsilon^2 C_{h2}, \quad (3.4.7) \]
\[ C_V \sim C_{v0} + \epsilon C_{v1} + \epsilon^2 C_{v2}, \quad (3.4.8) \]
\[ \Psi_s \sim \Psi_{s0} + \epsilon \Psi_{s1} + \epsilon^2 \Psi_{s2}. \quad (3.4.9) \]

Substituting these expansions into the equations (3.3.5)–(3.3.7) collecting terms at each order, it is straightforward to find the solutions on the bulk diffusion timescale. As mentioned above the problem is singularly perturbed. Thus these outer solutions will involve constants which need to be determined by matching solutions obtained from the rescaling of the problem to the initial layer.

3.4.2.1 Leading order equations

The leading order equations are

\[ \Psi_{s0} = 0, \quad (3.4.10) \]
\[ \frac{dC_{v0}}{d\tau} = 0, \quad (3.4.11) \]
\[ \Psi_{s0} = 0, \quad (3.4.12) \]

As expected we see that \( \Psi_{s0} = 0 \). Solving the second equation we find that

\[ C_{v0}(\tau) = K_1 e^{-\tau}. \quad (3.4.13) \]

3.4.2.2 Order \( \epsilon \) equations

Substituting in the known terms, the order \( \epsilon \) equations are

\[ \frac{dC_{h0}}{d\tau} = \frac{b_2}{b_1} \Psi_{s1} + K_1 e^{-\tau}, \quad (3.4.14) \]
\[ \frac{dC_{v1}}{d\tau} = b_1 C_{h0} - C_{v1}, \quad (3.4.15) \]
\[ \Psi_{s1} = 0. \quad (3.4.16) \]
3.4 Model analysis and asymptotic solutions

Once again we see immediately that $\Psi_{s1} = 0$. Solving the remaining two equations we find that

$$C_{h0}(\tau) = K_2 - K_1 e^{-\tau},$$  \hspace{1cm} (3.4.17)

$$C_{v1}(\tau) = b_1 e^{-\tau}(K_2 e^{\tau} - K_1\tau) - K_3 e^{-\tau}. \hspace{1cm} (3.4.18)$$

3.4.2.3 Order $\epsilon^2$ equations

Substituting in the known terms, the order $\epsilon^2$ equations are

$$\frac{dC_{h1}}{d\tau} = \frac{b_2}{b_1} \Psi_{s2} + K_1 b_1 e^{-\tau} - K_1 b_1 \tau e^{-\tau} + K_3 e^{-\tau},$$  \hspace{1cm} (3.4.19)

$$\frac{dC_{v2}}{d\tau} = b_1 (K_2 - K_1 e^{-\tau}) - C_{v2},$$  \hspace{1cm} (3.4.20)

$$\Psi_{s2} = 0. \hspace{1cm} (3.4.21)$$

Solving the non-trivial equations we find that

$$C_{h1}(\tau) = e^{-\tau}(b_1 K_1\tau - K_3) + K_4, \hspace{1cm} (3.4.22)$$

$$C_{v2}(\tau) = b_1 e^{-\tau} \left( \frac{1}{2} b_1 K_1\tau^2 - K_3\tau + K_4 e^{\tau} \right) + K_5 e^{-\tau}. \hspace{1cm} (3.4.23)$$

3.4.2.4 Outer solutions

Collecting the outer solutions we have

$$C_h(\tau) = K_2 - K_1 e^{-\tau} + \epsilon \left( e^{-\tau}(b_1 K_1\tau - K_3) + K_4 \right), \hspace{1cm} (3.4.24)$$

$$C_v(\tau) = K_1 e^{-\tau} + \epsilon \left( b_1 e^{-\tau}(K_2 e^{\tau} - K_1\tau) - K_3 e^{-\tau} \right)$$

$$+ \epsilon^2 \left( b_1 e^{-\tau} \left( \frac{1}{2} b_1 K_1\tau^2 - K_3\tau + K_4 e^{\tau} \right) + K_5 e^{-\tau} \right), \hspace{1cm} (3.4.25)$$

$$\Psi_s(\tau) \equiv 0, \hspace{1cm} (3.4.26)$$

where $K_1$–$K_5$ are constants to be determined by matching with the inner. The outer solution for $\Psi_s(\tau)$ is identically zero.
3. COFFEE EXTRACTION IN A WELL MIXED SYSTEM

3.4.3 Perturbation solutions on the surface dissolution (inner) timescale

In this section we will consider the system behaviour in the initial layer. To do this we rescale time to the fast timescale, by introducing an initial layer coordinate 
\( t = \frac{\tau}{\epsilon} \). We also rescale \( c_h^* \) and to account for the different balances in the system in the initial layer. In particular the concentration scale for \( c_h \) is chosen to balance the rate of change of concentration with the surface dissolution term. The scale for \( \psi_s^* \) is again chosen as its initial value. Specifically we rescale the system as follows:

\[
\tau = \epsilon t, \quad C_h(\tau) = \frac{b_2}{b_1} c_h(t), \quad (3.4.27)
\]

\[
C_v(\tau) = c_v(t), \quad \Psi_s(\tau) = \psi_s(t). \quad (3.4.28)
\]

The scales for each of the dimensional variables in the initial layer are

\[
\begin{align*}
&c_h^* \sim \frac{c_s^* (1 - \phi_h)}{r_s \phi_h}, & \quad & c_v^* \sim c_{\text{sat}}, \\
&t^* \sim t_s = \frac{c_s^* k_s m}{12 \beta^* c_{\text{sat}} D_h \phi_c r_s}, & \quad & \psi_s^* \sim \psi_{s0} = 1.
\end{align*} \quad (3.4.29) \quad (3.4.30)
\]

Thus the equations on the inner timescale are given by:

\[
\begin{align*}
\frac{dc_h}{dt} &= -\epsilon b_2 c_h \psi_s + \psi_s - \epsilon^2 b_1 c_h + \epsilon \frac{b_1}{b_2} c_v, \quad (3.4.31) \\
\frac{dc_v}{dt} &= \epsilon^2 b_2 c_h - \epsilon c_v, \quad (3.4.32) \\
\frac{d\psi_s}{dt} &= \epsilon b_2 c_h \psi_s - \psi_s, \quad (3.4.33)
\end{align*}
\]

\[
\begin{align*}
c_h(0) &= 0, & \quad & c_v(0) = \gamma_1, & \quad & \psi_s(0) = 1. \quad (3.4.34)
\end{align*}
\]

It is apparent that at leading order on the fast timescale \( \psi_{s0} \) decays exponentially, while \( c_v \) is constant. To find the solutions in detail we use the following
regular expansions for the surface dissolution timescale:

\[ c_h \sim c_{h0} + \epsilon c_{h1} + \epsilon^2 c_{h2}, \]  
(3.4.35)

\[ c_v \sim c_{v0} + \epsilon c_{v1} + \epsilon^2 c_{v2}, \]  
(3.4.36)

\[ \psi_s \sim \psi_{s0} + \epsilon \psi_{s1} + \epsilon^2 \psi_{s2}. \]  
(3.4.37)

### 3.4.3.1 Leading order equations

The leading order equations are

\[ \frac{d c_{h0}}{dt} = \psi_{s0}, \]  
(3.4.38)

\[ \frac{d c_{v0}}{dt} = 0, \]  
(3.4.39)

\[ \frac{d \psi_{s0}}{dt} = -\psi_{s0}, \]  
(3.4.40)

\[ c_{h0}(0) = 0, \quad c_{v0}(0) = \gamma_1, \quad \psi_{s0}(0) = 1. \]  
(3.4.41)

Solving these equations we find that

\[ c_{h0}(t) = 1 - e^{-t}, \]  
(3.4.42)

\[ c_{v0}(t) = \gamma_1, \]  
(3.4.43)

\[ \psi_{s0}(t) = e^{-t}. \]  
(3.4.44)

### 3.4.3.2 Order \( \epsilon \) equations

The order \( \epsilon \) equations are

\[ \frac{d c_{h1}}{dt} = \psi_{s1} - b_2 c_{h0} \psi_{s0} + \frac{b_1}{b_2} c_{v0}, \]  
(3.4.45)

\[ \frac{d c_{v1}}{dt} = -c_{v0}, \]  
(3.4.46)

\[ \frac{d \psi_{s1}}{dt} = b_2 c_{h0} \psi_{s0} - \psi_{s1}, \]  
(3.4.47)

\[ c_{h1}(0) = 0, \quad c_{v1}(0) = 0, \quad \psi_{s1}(0) = 0. \]  
(3.4.48)
Substituting in the leading order solutions we can solve these equations to obtain

\[ c_{h1}(t) = \frac{b_1 \gamma_1 t}{b_2} + b_2 e^{-2t} (-c^t(t-1) - 1), \]
\[ c_{v1}(t) = -\gamma_1 t, \]
\[ \psi_{s1}(t) = b_2 e^{-2t} (c^t(t-1) + 1). \]

### 3.4.3.3 Order $\epsilon^2$ equations

The order $\epsilon^2$ equations are

\[ \frac{dc_{h2}}{dt} = \psi_{s2} - b_2 (c_{h1} \psi_{s0} + c_{h0} \psi_{s1}) + b_1 c_{h0} + \frac{b_1}{b_2} c_{v1}, \]
\[ \frac{dc_{v2}}{dt} = b_2 c_{h0} - c_{v1}, \]
\[ \frac{d\psi_{s2}}{dt} = b_2 (c_{h1} \psi_{s0} + c_{h0} \psi_{s1}) - \psi_{s2}, \]

\[ c_{h2}(0) = 0, \quad c_{v2}(0) = 0, \quad \psi_{s2}(0) = 0. \]

Substituting in the known terms we can solve the equations to obtain

\[ c_{h2}(t) = \frac{e^{-3t} \left(-b_1 b_2 e^{2t} (\gamma_1 t^2 + 2 c^t(t-1) + 2)\right)}{b_2} \]
\[ + \frac{e^{-3t} \left(-b_1 \gamma_1 e^{3t} t^2 - b_2^2 \left(c^t(t-2)t + 4t - 2\right) + 2\right)}{2b_2}, \]
\[ c_{v2}(t) = e^{-3t} \left(b_1 \gamma_1 e^{2t} t^2 + b_2^2 \left(c^t(t-2)t + 4t - 2\right) + 2\right), \]
\[ \psi_{s2}(t) = \frac{1}{2} \left(e^{-3t} \left(b_1 \gamma_1 e^{2t} t^2 + b_2^2 \left(c^t(t-2)t + 4t - 2\right) + 2\right)\right). \]
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3.4.3.4 Inner solutions

Collecting the solutions of each order we have the following inner solutions:

\[ c_h(t) = e^{-t} (e^t - 1) + \epsilon \left( \frac{b_1 \gamma_1 t}{b_2} + b_2 e^{-2t} (-e^t (t - 1) - 1) \right) \]
\[ + \epsilon^2 \left( \frac{e^{-3t} \left( -b_1 b_2 e^{2t} (\gamma_1 t^2 + 2e^t (t - 1) + 2) \right) \gamma_1 t^2}{2b_2} \right) \]  
\[ + \frac{e^{-3t} \left( -b_1 \gamma_1 e^{3t} t^2 - \gamma_1^2 t^2 + b_2^3 \left( e^{t} (e^t (t - 2) t + 4t - 2) + 2 \right) \right)}{2b_2}, \]  
\[ (3.4.59) \]

\[ c_v(t) = \gamma_1 - \epsilon (\gamma_1 t) + \epsilon^2 \left( b_2 \left( t + e^{-t} - 1 \right) + \frac{\gamma_1 t^2}{2} \right), \]  
\[ (3.4.60) \]

\[ \psi_s(t) = -b_1 \gamma_1 e^{-t} + \epsilon \left( b_2 e^{-2t} \left( e^t (t - 1) + 1 \right) \right) \]
\[ + \frac{1}{2} \epsilon^2 \left( e^{-3t} \left( b_1 \gamma_1 e^{2t} t^2 + b_2 \left( e^t (e^t (t - 2) t + 4t - 2) + 2 \right) \right) \right) \].  
\[ (3.4.61) \]

3.4.4 Matching

The integration constants in the outer solutions can be determined by matching these solutions with the initial layer solutions. We do this using modified Van Dyke matching [71]. In this method we compare the inner expansion of the outer solutions with the outer expansion of the inner solutions to obtain the unknown constants \( K_1 - K_5 \). Applying this method we find that

\[ K_1 = \gamma_1, \quad K_2 = \frac{b_2}{b_1} + \gamma_1, \quad K_3 = -b_1 \gamma_1 - b_2, \]  
\[ (3.4.62) \]

\[ K_4 = -b_1 \gamma_1 - b_2, \quad K_5 = \frac{b_2}{b_1} \gamma_1 + b_2 b_1 - b_2. \]  
\[ (3.4.63) \]

The matched outer solutions are

\[ C_h(\tau) = \frac{b_2}{b_1} - \gamma_1 e^{-\tau} + \gamma_1 + \epsilon \left( e^{-\tau} (b_1 \gamma_1 (\tau + 1) + b_2) - (b_1 \gamma_1 + b_2) \right), \]  
\[ (3.4.64) \]

\[ C_v(\tau) = \gamma_1 e^{-\tau} + \epsilon \left( e^{-\tau} (b_1 \gamma_1 e^\tau - b_1 \gamma_1 \tau + b_2 e^\tau) - e^{-\tau} (b_1 \gamma_1 + b_2) \right) \]
\[ + \frac{\epsilon^2 \left( b_1^2 \gamma_1 + b_1 b_2 - b_2 \right)}{2} \]
\[ - b_1 \gamma_1 e^{-\tau} \left( \frac{1}{2} b_1 \gamma_1 \tau^2 - b_1 \gamma_1 \tau + b_1 \gamma_1 e^\tau - b_2 \tau + b_2 e^\tau \right), \]  
\[ (3.4.65) \]

\[ \Psi_s(\tau) = 0. \]  
\[ (3.4.66) \]
3. COFFEE EXTRACTION IN A WELL MIXED SYSTEM

Thus the composite solutions on the inner timescale and concentration scale are

\[ c_{h\text{comp}}(t) = c_h(t) + \frac{b_1}{b_2} C_h(\epsilon t) - \frac{\epsilon^2 \left(-b_1 b_2 t - \frac{1}{2} b_1 \gamma_1 t^2\right)}{b_2} + b_1 \gamma_1 t \epsilon + b_2, \quad (3.4.67) \]

\[ c_{v\text{comp}}(t) = c_v(t) + C_v(\epsilon t) - \left(\epsilon^2 \left(b_2 t - b_2 + \frac{\gamma_1 t^2}{2}\right) + \gamma_1 - \gamma_1 t \epsilon\right), \quad (3.4.68) \]

\[ \psi_{s\text{comp}}(t) = \psi_s(t). \quad (3.4.69) \]

3.4.5 Comparison of Asymptotics with Numerical Simulation

The composite solutions are compared with the numerical solution of equations (3.4.31)–(3.4.34) and available experimental data in figure 3.2. The comparison with data is shown for two different grind size distributions from ref. [51]: one fine grind called JK drip filter grind and one relatively coarse grind called Cimbali #20 grind. Available data for coffee concentration in the intergranular fluid is compared to the approximate and numerical solutions based on the parameters for these two grinds. The asymptotic and numerical solutions to the model for intragranular concentration \( c_v(t) \) and the fraction of coffee remaining on the grain surfaces \( \psi_s(t) \) are also plotted. No data is available for comparison in this case.

3.5 Conclusion

In this chapter the mathematical model of coffee extraction described in chapter 2 is analysed. The model equations are simplified and non-dimensionalised to describe extraction of coffee from a dilute suspension of coffee grains. The dimensionless form of the equations represents a much simpler description of the important processes in this situation and depends on a much smaller set of parameters than the original equations. This is a good example of model reduction [63]. Approximate solutions of the specialised dimensionless equations can be found using perturbation techniques. These solutions depend on dimensionless parameters which are defined in terms of the physical parameters of the system. Thus the approximate solutions are useful to both quickly fit solutions to a particular set of process parameters and to investigate the influence of changing a particular parameter on the system.
3.5 Conclusion

The model equations used to describe the extraction of coffee in a fixed volume admit approximate solutions due to the existence of two different extraction mechanisms over difference timescales. Extraction of coffee from the surfaces of the coffee grains proceeds much faster than diffusion of coffee through the intragranular pore network to the grain surface. The ratio of these timescales gives us a small non-dimensional parameter. We utilise this parameter to form solutions on the inner (surface dissolution) and outer (diffusion from grain kernel) timescales based on the dominant mechanisms in these regimes. These approximate solutions are found to match the numerical solutions well and provide a much simpler equation to fit to data.

Extraction of coffee solubles from individual coffee grains is a key operation in many brewing techniques. The physical description of extraction here is observed to describe extraction well in the case of extraction from a dilute suspension of coffee grains. Thus it may be useful in models of more complicated brewing techniques to describe the grain extraction kinetics component of the procedure. This will be shown in the case of extraction in flow through a packed coffee bed in chapter 4. On the scale of a coffee grain there is scope to investigate the dissolution of coffee within a coffee grain in more detail to investigate some of the assumptions made in this chapter.
Figure 3.2: Comparison of numerical and approximate solutions for fine and coarse grinds: Comparison of numerical (--) and composite (−) solutions for (a) $c_h(t)$ (Experimental data points are included), (b) $c_v(t)$ and (c) $\psi_s(t)$ for $\epsilon = 0.028$, $b_1 = 5.239$, $b_2 = 2.897$ and $\gamma_1 = 0.70$ (JK drip filter grind). Plots (d), (e) and (f) show the corresponding results for $\epsilon = 0.071$, $b_1 = 1.99$, $b_2 = 1.35$ and $\gamma_1 = 0.5$ (Cimbali #20 grind).
CHAPTER 4

COFFEE EXTRACTION IN A PACKED COFFEE BED

4.1 Introduction

In chapter 2 a general double porosity model of coffee extraction in a fixed coffee bed was presented. Making certain assumptions, it was shown that the model could reproduce experimentally measured extraction curves for extraction of coffee from a cylindrical brewing chamber. The experimental set-up and data collected is described in section 2.2.4. Despite being based on a number of simplifying assumptions the model equations for this situation could only be solved numerically. In this chapter we consider the model reduction of the general equations in detail and analyse the specialised model equations. The system of equations is non-dimensionalised to identify the dominant mechanisms during coffee extraction. Approximate solutions can be found based on the dominant mechanism of extraction during different stages of the brewing process. Solutions can be found for both fine and coarse grinds in the two experimental situations outlined in section 2.2.4. Based on these experiments, this chapter focuses on developing approximate solutions for coffee extraction from a flow-through cylinder similar to that found in an espresso machine, except the water is at a much lower pressure. In this case, solutions for extraction of fine and course grinds differ due to a difference in the assumed initial coffee concentration in the coffee bed. Solu-
4. COFFEE EXTRACTION IN A PACKED COFFEE BED

...tions are presented for both fine and coarse grind parameters. Such solutions can be used to predict the coffee quality (coffee concentration and extraction yield) for a particular brewing configuration with a given set of process parameters.

4.1.1 General coffee extraction model

As in chapter 3, we begin with the general coffee extraction model comprising equations (2.6.51)–(2.6.57). In this section we will consider the one-dimensional form of the general equations for a coffee bed of height \( L \). The key assumptions made in finding the numerical solution to the equations in section 2.8.2 will be expanded on and discussed. The reduction of the equations to one spatial dimension is possible due to the cylindrical geometry of the coffee bed and nature of the flow, which allows us to assume that the coffee bed properties are homogeneous in any cross section. Thus the spatial dimension is the coffee bed depth, which we label with the \( z \)-coordinate. The height of the coffee bed is \( L \), with the bottom (filter exit) at \( z = 0 \) and the top (filter entrance) at \( z = L \). As in chapter 3 we neglect the term for transfer of fluid between the h-phase and v-phase due to differences in pressures. This correction is thought to occur much faster than other bed processes. Here the ad-hoc assumption is made that \( p_h = p_v \) in the equations. Physically this assumption should have only a small influence in our results as the change in porosity due to coffee dissolution following filling is small. Careful asymptotic analysis should reveal a small reduction in the Darcy velocity while the intragranular porosity is changing, but this will not be outlined here. Neglecting the term here means we assume that solid coffee and water occupy the same space as that coffee dissolved in the water. As coffee diffuses out of the grain the water needed to replace that coffee is not accounted for in the model. For these reasons the coffee solution transfer terms are neglected in the presentation...
of the equations here. Thus the general one-dimensional model becomes:

\[
\frac{\partial c^*_h}{\partial t^*} = \frac{k^2_s}{36\kappa \mu (1-\phi_h)^2} \frac{\partial}{\partial z^*} \left( c^*_h \left( \frac{\partial p^*_h}{\partial z^*} + \rho g \right) \right) + \frac{1}{2} D_h \frac{\partial^2 c^*_h}{\partial z^{*2}}
\]

\[+ D_v \frac{\partial^2 c^*_h}{\partial z^{*2}} - \alpha^* (1-\phi_h) \frac{\phi_v^*}{\phi_h} \frac{4}{3} D_v \frac{6}{k_{sv2} l} (c^*_h - c^*_v)
\]

\[+ \beta^* (1-\phi_h) \frac{12 D_h \phi_{cd}}{k_{sv1} m} (c_{sat} - c^*_h) \psi^*_s,
\]

\[\frac{\partial^2 p^*_h}{\partial z^{*2}} = 0,
\]

\[\frac{\partial c^*_v}{\partial t^*} = \alpha^* \phi_v^* \frac{4}{3} D_v \frac{6}{k_{sv2} l} (c^*_h - c^*_v) + \gamma^* \phi_v^* \frac{12 \phi_{cd} D_v}{m^2} (c_{sat} - c^*_v) \psi^*_v
\]

\[- \frac{c^*_v}{\phi_v^*} \frac{\partial \phi_v^*}{\partial t^*},
\]

\[\frac{\partial \phi_v^*}{\partial t^*} = -\frac{1}{r_s} \frac{\partial \psi^*_s}{\partial t^*} - \frac{1}{r_v} \frac{\partial \psi^*_v}{\partial t^*},
\]

\[\frac{\partial \psi^*_s}{\partial t^*} = -\beta^* \frac{12 D_h \phi_{cd}}{k_{sv1} m} \left( \frac{c_{sat} - c^*_h}{c_s} \right) r_s \psi^*_s,
\]

\[\frac{\partial \psi^*_v}{\partial t^*} = -\gamma^* \frac{12 D_v \phi_{cd}}{m^2} \left( \frac{c_{sat} - c^*_v}{c_s} \right) r_v \psi^*_v.
\]

\[0 < z^* < L, \quad t^* > 0,
\]

\[c^*_h(z^*, 0) = c^*_h(0, z^*), \quad c^*_v(z^*, 0) = c^*_v(0, z^*),
\]

\[\phi_v^*(z^*, 0) = \phi_v^*(0, z^*), \quad \psi^*_s(z^*, 0) = \psi^*_s(0, z^*), \quad \psi^*_v(z^*, 0) = \psi^*_v(0, z^*).
\]

\[p^*_h(0, t^*) = 0, \quad p^*_h(L, t^*) = \Delta P, \quad c^*_h(L, t^*) = 0, \quad \frac{\partial c^*_h(0, t^*)}{\partial z^*} = 0.
\]

The pressure boundary conditions come from the recorded pressure drop in experiment. The concentration in the incoming water is zero at the inlet and it is assumed that the diffusive flux is zero at the outlet. Initial conditions need to be determined or inferred from experiment once the bed is saturated with water, following the initial addition of water to the dry coffee bed. The initial conditions could also be determined by modelling the unsaturated flow during the initial infiltration of water. This is investigated in chapter 5. Note as in chapter 3 the presence experimental fitting parameters, \(\alpha^*, \beta^*\) and \(\gamma^*\), for the
mass transfer terms. These parameters are used to fit the model to experiment. These are required because many of the parameters in the model are difficult to obtain. The fitting parameters account for errors in each of the components of their respective mass transfer coefficients.

4.2 Model specialisation

Before non-dimensionalising the system we can take some further simplifying steps. Equation (4.1.2) can be solved using the pressure boundary conditions from the experiment in question, to find \( p^*_h = \frac{\Delta P}{L} z^* \). Substituting this into (4.1.1) eliminates \( p^*_h \). Integrating equation (4.1.4) with respect to time we see that:

\[
\phi^*_v + \frac{1}{r_s} \psi^*_s + \frac{1}{r_v} \psi^*_v = f(z),
\]

where \( f(z) \) is an arbitrary function of \( z \). We note that this is just the sum of the intragranular pore volume fraction, the volume fraction of solid coffee on the surface and the volume fraction of solid coffee in the grain kernels. This sum must be equal to the maximum intragranular pore volume fraction (porosity) which we define as \( \phi^*_v \) and corresponds to the situation in which all soluble coffee is dissolved. The value of \( \phi^*_v \) can be estimated from data on the percentage of the coffee grain mass which is soluble for a given coffee grind. Thus we can eliminate \( \phi^*_v \) from the system using (4.1.4) and

\[
\phi^*_v = \phi^*_v - \frac{1}{r_s} \psi^*_s - \frac{1}{r_v} \psi^*_v.
\]

However this still leaves us with quite a complex system to analyse. To further simplify we assume that the volume fraction of coffee in the grains is small compared to the final intragranular porosity. This corresponds to \( \phi_{s,ad} + \phi_{s,bd} = r_s^{-1} + r_v^{-1} \ll \phi^*_v \). Thus we make the approximation that \( \phi^*_v \approx \phi^*_v \) in the equations. We need to account for this when assigning initial conditions in the intragranular pores.

In order to use the model we need to find values for \( \alpha^* \), \( \beta^* \) and \( \gamma^* \). Experimental extraction profiles are available for \( c^*_h \) at the filter exit and the two rates of extraction are evident in the profiles. Thus \( \alpha^* \) and \( \beta^* \) can be fitted. Data is not available for \( c^*_v \) however so \( \gamma^* \) cannot be determined. A reasonable approximation
may be that $\gamma^* \approx \beta^*$. In reality due to a much larger surface area per unit volume within the volume it is likely that $\gamma^* > \beta^*$. Dissolution of coffee within the coffee grain and diffusion of coffee from the grain pore network occur consecutively. Based on the assumption that $\gamma^* \geq \beta^*$ diffusion of coffee is the rate limiting step in this series. We expect dissolution within the grains to proceed at a similar rate to dissolution from grain surfaces, but experiments show a much slower extraction from the grains so the diffusion limited assumption seems reasonable. Thus to simplify the analysis, we assume the solid coffee in the cell walls within the grains dissolves into the intragranular pores very quickly initially so that all soluble coffee in the grains is dissolved in the fluid in the intragranular pores initially (i.e. once the coffee bed is saturated with water). The validity of this assumption is based on the timescale of the dissolution process being much shorter than the grain diffusion timescale. Provided that diffusion of coffee from the grains is the rate limiting step of extraction, rather than solid dissolution within the grains, the model may still work quite well. This corresponds to $\psi^*_v(z^*, 0) = 0$ and means equation (4.1.6) drops out. This also allows us to estimate $c^*_v(z^*, 0)$ by assuming all the soluble coffee in the grain kernels has dissolved in the intragranular pores. Thus we let $c^*_v(z^*, 0) = \eta c_{sat}$ with $0 \leq \eta \leq 1$ depending on the coffee grind in question. The unsaturated flow during the initial infiltration of water into the dry bed is not modelled here. This means we need to estimate the remaining initial conditions after the bed is saturated with water and coffee brew starts to exit at the bottom. Experiments suggest that the exiting coffee concentration may be steady for perhaps the first wash through of the coffee bed before it starts to drop. Initial exiting concentration for fine grinds is significantly higher than for coarser grinds and may be close to the solubility of coffee in water. Based on the experiment data it will be assumed that the initial concentration profile for the fine grind considered is at coffee solubility throughout the bed so $c^*_h(z^*, 0) = c_{sat}$. For coarser grinds a linear initial coffee concentration profile will be assumed, varying from 0 at the filter entrance to the initial exiting concentration from experiments $c_{max}$ at the filter exit. So for coarser grinds $c^*_h(z^*, 0) = c_{max} \frac{(L-z^*)}{L}$. More generally it would be useful to find approximate solutions for an initial concentration profile which is an arbitrary function of $z^*$, $h^*(z^*)$. It remains to assign the initial condition to $\psi^*_s(z^*, 0)$, which represents the fraction of the initial volume fraction of soluble coffee on the grain surfaces remaining following water infiltration. One would expect this term to be smaller at the top of the bed than at the bottom.
since water is in contact with these grinds for longer during infiltration. However without modelling the initial water infiltration the simplest assumption is to uniformly decrease \(\psi_s^*(z^*,0)\) to correspond to the amount of coffee which has dissolved to give \(c_h^*(z^*,0)\). Thus we let \(\psi_s^*(z^*,0) = \psi_{s0}^*\) with \(0 \leq \psi_{s0}^* \leq 1\). \(\psi_{s0}^*\) depends on the parameters of the coffee grind in question and the assumed initial concentration profile. With all this in mind, we rewrite the dimensional equations as:

\[
\frac{\partial c_h^*}{\partial t^*} = \frac{k_{sv1}^2 \phi_h^2}{36 \kappa \mu (1 - \phi_h)^2} \left(\frac{\Delta P}{L} + \rho g\right) \frac{\partial c_h^*}{\partial z^*} + \frac{1}{\phi_h} D_h \frac{\partial^2 c_h^*}{\partial z'^2} \\
+ D_h^h \frac{\partial^2 c_h^*}{\partial z'^2} - \alpha^* \frac{(1 - \phi_h)}{\phi_h} \phi_v^\infty \frac{D_v}{k_{sv2} t} (c_h^* - c_v^*) \\
+ \beta^* \frac{(1 - \phi_h)}{\phi_h} 12 D_h \phi_{cd} (c_{sat} - c_h^*) \psi_s^*,
\]

\[
\frac{\partial c_v^*}{\partial t^*} = \alpha^* \phi_v^\infty \frac{1}{\phi_h} \frac{D_v}{k_{sv1} m} (c_h^* - c_v^*) \\
\frac{\partial \psi_s^*}{\partial t^*} = -\beta^* \frac{12 D_h \phi_{cd}}{k_{sv1} m} \left(\frac{c_{sat} - c_h^*}{c_s}\right) r_s \psi_s^*.
\]

\[
0 < z^* < L, \quad t^* > 0,
\]

\[
c_h^*(z^*,0) = h^*(z^*), \quad c_v^*(z^*,0) = \eta c_{sat}, \quad \psi_s^*(z^*,0) = \psi_{s0}^*.
\]

\[
c_h^*(L,t^*) = 0, \quad \frac{\partial c_h^*(0,t^*)}{\partial z^*} = 0.
\]

We also have \(\psi_v^*(z^*,t^*) = 0\) and \(\phi_v^*(z^*,t^*)\) is given by equation (4.2.2). A summary of the model parameters and values for fine and coarse grinds is given in tables 4.1 and 4.2. The solution here will depend on the initial conditions for a fine coffee grind \(h^*(z^*) = h_f^*(z^*) = c_{sat}\) and for a coarse coffee grind \(h^*(z^*) = h_c^*(z^*) c_{max} \frac{(L - z^*)}{L}\), as outlined above. We will proceed with the solution for the general initial condition \(h^*(z^*)\) before specialising to coarse and fine grinds.
4.2 Model specialisation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi^\infty$</td>
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<td>$\phi_h$</td>
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<td>$\beta^*$</td>
<td>surface dissolution fitting coefficient</td>
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<tr>
<td>$k_{sv2}$</td>
<td>Sauter mean diameter (grains &gt; 50 µm)</td>
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<td>$l_l$</td>
<td>mean volume weighted grain radius</td>
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<td>coffee diffusion coefficient (for caffeine)</td>
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<td>965.3 kg m$^{-3}$</td>
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<tr>
<td>$\mu$</td>
<td>liquid viscosity (for water at 90 °C)</td>
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<tr>
<td>$m$</td>
<td>coffee cell diameter</td>
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<td>$g$</td>
<td>acceleration due to gravity</td>
<td>9.81 m s$^{-2}$</td>
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Table 4.1: Parameters for cylindrical brewing chamber extraction experiments with JK drip filter grind.

4.2.1 Non-dimensionalisation

For the parameters involved in the extraction experiments for either the coarse or fine coffee grinds the advection term is found to dominate strongly over the diffusion and mechanical dispersion terms in equation (4.2.3). To see this we consider the ratio of the advection term to the diffusion term (with $z^* \sim L$) for the coffee flow-through cell which is given by

$$\frac{k_{sv1}^2 L \phi_h^5}{36 \kappa \mu D_h (1 - \phi_h)^2} \left( \frac{\Delta P}{L} + \rho g \right)$$  (4.2.9)

For the experiments in question here we have $\frac{\Delta P}{L} \gg \rho g$ so the ratio is approximately given by

$$\frac{k_{sv1}^2 \Delta P \phi_h^5}{36 \kappa \mu D_h (1 - \phi_h)^2}$$  (4.2.10)
4. COFFEE EXTRACTION IN A PACKED COFFEE BED

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Value</th>
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<td>$\phi_h$</td>
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<td>soluble coffee volume fraction</td>
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<td>$k_{sv1}$</td>
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<td>Sauter mean diameter (grains $&gt;$ 50µm)</td>
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<td>$l_t$</td>
<td>mean volume weighted grain radius</td>
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<tr>
<td>$D_h = D_v$</td>
<td>coffee diffusion coefficient (for caffeine)</td>
<td>$2.2 \times 10^{-9}$ m$^2$s$^{-1}$</td>
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<tr>
<td>$\rho$</td>
<td>liquid density (for water at 90°C)</td>
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</tr>
<tr>
<td>$\mu$</td>
<td>liquid viscosity (for water at 90°C)</td>
<td>$0.315 \times 10^{-3}$ Pa s</td>
</tr>
<tr>
<td>$m$</td>
<td>coffee cell diameter</td>
<td>30 µm</td>
</tr>
<tr>
<td>$c_{sat}$</td>
<td>coffee solubility</td>
<td>212.4 kg m$^{-3}$</td>
</tr>
<tr>
<td>$c_{max}$</td>
<td>coffee concentration at exit</td>
<td>82.63 kg m$^{-3}$</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>Kozeny-Carman shape coefficient</td>
<td>3.1</td>
</tr>
<tr>
<td>$\eta$</td>
<td>initial intragranular concentration level</td>
<td>0.5</td>
</tr>
<tr>
<td>$\psi_{s0}$</td>
<td>fraction of $\phi_{s,sd}$ remaining after filling</td>
<td>0.8595</td>
</tr>
<tr>
<td>$g$</td>
<td>acceleration due to gravity</td>
<td>9.81 m s$^{-2}$</td>
</tr>
</tbody>
</table>

Table 4.2: Parameters for cylindrical brewing chamber extraction experiments with Cimbali #20 grind.

We use the parameters from table 4.1 to estimate this term. Thus

$$\frac{k_{sv1}^2 \Delta P \phi_h^5}{36\kappa \mu D_h (1 - \phi_h)^2} \sim 10^7,$$

and so advection dominates strongly over diffusion. Similarly the ratio of advection to dispersion is

$$\frac{k_{sv1}^2 L \phi_h^2}{36\kappa \mu D^b (1 - \phi_h)^2} \left( \frac{\Delta P}{L} + \rho g \right) \approx \frac{k_{sv1}^2 \Delta P \phi_h^2}{36\kappa \mu D^b (1 - \phi_h)^2}.$$

The dispersion coefficient is more difficult to estimate and is related to the pore size and the fluid velocity in the pores. In section 2.6.8, a general expression for the dispersion coefficient in terms of fluid velocity and average pore size is
used to show the dominance of advection. Here we just note that unless the dispersion coefficient is many orders of magnitude greater in size than the diffusion coefficient, advection dominates over dispersion. For this reason these terms are neglected.

There are three main timescales of interest in the model. The timescale over which coffee diffuses from the grain kernels to the intergranular pores is referred to as the bulk diffusion timescale \( t_d \). The timescale over which the coffee dissolves from the grain surfaces into the intergranular pores is referred to as the surface dissolution timescale \( t_s \). Finally the timescale over which the coffee solubles are carried in the flow out of the bed is referred to as the advection timescale \( t_a \). In terms of the coffee bed parameters, these timescales are defined as:

\[
\begin{align*}
  t_d &= \frac{k_{sv2}l_t}{6\alpha^*\phi_c^{\frac{1}{3}}D_v}, \\
  t_s &= \frac{k_{sv1}m\phi_h}{12\beta^*D_h\phi_{cd}\psi_{st}(1-\phi_h)}, \\
  t_a &= \frac{36L^2\kappa\mu(1-\phi_h)^2}{k_{sv1}\phi_h^2(\Delta P + \rho g L)}.
\end{align*}
\]

(4.2.13)

For the fine grind parameters given in table 4.1, \( t_s = 1.042 \) s, \( t_a = 5.356 \) s and \( t_d = 42.231 \) s. For the coarse grind parameters \( t_s = 10.26 \) s, \( t_a = 8.891 \) s and \( t_d = 246.972 \) s. First we scale the equations on the bulk diffusion timescale. The concentration scale for the intergranular pores is chosen to balance the advection term with the transfer of coffee solubles by diffusion from the grains. The scale for the \( \psi_s^* \) is chosen so that the source term for transfer of coffee from the surface balances the previous two terms. The scales chosen are as follows

\[
\begin{align*}
  c_h^* &\sim \frac{216\kappa\mu L^2\alpha^*\delta_c \phi_c^{\frac{1}{3}}(1-\phi_h)^3}{k_{sv2}k_{sv1}\phi_h^2l_t(\Delta P + \rho g L)} c_{sat}, \\
  c_v^* &\sim c_{sat}, \\
  t^* &\sim t_d = \frac{k_{sv2}l_t}{6\alpha^*\phi_c^{\frac{1}{3}}D_v}, \\
  \psi_s^* &\sim \frac{\alpha^*\delta_v\phi_v^{\frac{1}{2}}k_{sv1}m}{2\beta^*D_h\phi_{cd}k_{sv2}l_t}, \\
  z^* &\sim L.
\end{align*}
\]

(4.2.14)

Before we present the non-dimensional equations on the bulk diffusion timescale, we define some non-dimensional parameters to tidy up the presentation. First we define \( \epsilon \) to be the ratio of the advection timescale to the timescale of diffusion of coffee from the grains. Thus

\[
\epsilon = \frac{216\kappa\mu L^2\alpha^*\delta_c \phi_c^{\frac{1}{3}}(1-\phi_h)^2}{k_{sv2}k_{sv1}\phi_h^2l_t(\Delta P + \rho g L)} = \frac{t_a}{t_d}.
\]

(4.2.16)
4. COFFEE EXTRACTION IN A PACKED COFFEE BED

The other three non-dimensional parameters are given by

\[ a_1 = \frac{1 - \phi_h \phi_v}{\phi_h}, \quad a_2 = \frac{432 \kappa \mu L^2 \beta^* D_h \phi_v \psi_{s0}^* (1 - \phi_h)^3}{k_{sv1} m \phi_h^3 (\Delta P + \rho g L)} = \frac{t_a}{t_s}, \quad a_3 = \frac{c_{sat} r_s \phi_h}{c_s (1 - \phi_h) \psi_{s0}^*}. \]  

(4.2.17)

Physically, \( a_1 \) represents the ratio of the intragranular volume to the intergranular volume, \( a_2 \) represents the ratio of the advection timescale to the surface dissolution timescale, and \( a_3 \) represents the ratio of the maximum coffee mass capacity of the intergranular pores to the initial mass of coffee present on the grain surfaces. We will assume here that \( \epsilon \ll 1 \) while \( a_1, a_2, \) and \( a_3 \) are all \( O(1) \). For the fine grind parameters we have \( \epsilon = 0.127, a_1 = 2.81, a_2 = 5.139, a_3 = 0.473 \). For the coarse grind parameters we have \( \epsilon = 0.036, a_1 = 2.0461, a_2 = 0.866, a_3 = 0.84 \). In terms of these parameters the equations on the bulk diffusion timescale with boundary and initial conditions prescribed are

\[ \frac{\epsilon \partial C_h}{\partial \tau} = \frac{\partial C_h}{\partial z} - \epsilon a_1 C_h + C_v + (1 - a_1 \epsilon C_h) \Psi_s, \]  

(4.2.18)

\[ \frac{\partial C_v}{\partial \tau} = a_1 \epsilon C_h - C_v, \]  

(4.2.19)

\[ \frac{\epsilon \partial \Psi_s}{\partial \tau} = -a_2 a_3 (1 - a_1 \epsilon C_h) \Psi_s, \]  

(4.2.20)

\[ 0 < z < 1, \quad \tau > 0, \]  

(4.2.21)

\[ C_h(z, 0) = \frac{1}{a_1 \epsilon} h(z), \quad C_v(z, 0) = \eta, \]  

(4.2.22)

\[ \Psi_s(z, 0) = \frac{a_2 \psi_{s0}^*}{a_1 \epsilon}, \quad C_h(1, \tau) = 0. \]  

(4.2.23)

The function \( h(z) = \frac{1}{c_{sat}} h^*(L z) \) is given by \( h(z) = h_f(z) = 1 \) for fine grinds and \( h(z) = h_c(z) = \zeta (1 - z) \) for coarse grinds. The parameter \( \zeta = \frac{c_{max}}{c_{sat}} \) satisfies \( 0 < \zeta < 1 \). It is clear from the form of the equations that we have a singular perturbation problem. Thus we will need to consider the dynamics of the system on an initial layer in order to satisfy the initial conditions. First we will solve the outer equations using a regular expansion. Any constants of integration which arise will need to be matched to the initial layer solutions when they are found.
4.3 Asymptotic solutions

4.3.1 Perturbation solutions on the bulk diffusion (outer) timescale

We use the following expansions for the bulk diffusion timescale

\[ C_h \sim C_{h0} + \epsilon C_{h1} + \epsilon^2 C_{h2}, \]  
\[ C_v \sim C_{v0} + \epsilon C_{v1} + \epsilon^2 C_{v2}, \]  
\[ \Psi_s \sim \Psi_{s0} + \epsilon \Psi_{s1} + \epsilon^2 \Psi_{s2}. \]  

4.3.1.1 Leading order solutions

The leading order equations are

\[ \frac{\partial C_{h0}}{\partial z} = -C_{v0} - \Psi_{s0}, \]  
\[ \frac{\partial C_{v0}}{\partial \tau} = -C_{v0}, \]  
\[ \Psi_{s0} = 0, \]

with solutions

\[ C_{h0}(z, \tau) = -e^{-\tau} \int_1^z f_1(\xi) d\xi, \quad C_{v0}(z, \tau) = e^{-\tau} f_1(z), \quad \Psi_{s0}(z, \tau) = 0, \]  

where \( f_1(z) \) is an arbitrary function of \( z \) to be determined by matching.

4.3.1.2 Order \( \epsilon \) solutions

Substituting in the known terms and using \( \Psi_{s1} = 0 \) from the third equation in the first and second, the first order equations are

\[ \frac{\partial C_{h1}}{\partial z} = e^{-\tau} (1 - a_1) \int_1^z f_1(\xi) d\xi - C_{v1}, \]  
\[ \frac{\partial C_{v1}}{\partial \tau} = -C_{v1} - a_1 e^{-\tau} \int_1^z f_1(\xi) d\xi, \]  
\[ \Psi_{s1} = 0, \]
with solutions

\[ C_{h1}(z, \tau) = -e^{-\tau} \left( \int_1^z f_2(\xi) d\xi \right) - e^{-\tau} \left( a_1 \tau - a_1 + 1 \right) \left( \int_1^z \int_1^\lambda f_1(\xi) d\xi d\lambda \right), \]  

(4.3.11)

\[ C_{v1}(z, \tau) = e^{-\tau} f_2(z) - a_1 e^{-\tau} \tau \left( \int_1^z f_1(\xi) d\xi \right), \]  

(4.3.12)

\[ \Psi_{s1}(z, \tau) = 0, \]  

(4.3.13)

where \( f_2(z) \) is a second arbitrary function of \( z \) to be determined by matching.

### 4.3.1.3 Solutions for the bulk diffusion (outer) timescale

In summary we have the following outer solutions:

\[ C_h(z, \tau) = -e^{-\tau} \int_1^z f_1(\xi) d\xi \]  

(4.3.14)

\[ - e^{\tau} \left( e^{-\tau} \left( \int_1^z f_2(\xi) d\xi \right) \right) \]  

\[ - e^{\tau} \left( a_1 \tau - a_1 + 1 \right) \left( \int_1^z \int_1^\lambda f_1(\xi) d\xi d\lambda \right), \]  

\[ C_v(z, \tau) = e^{-\tau} f_1(z) \]  

(4.3.15)

\[ + e^{\tau} f_2(z) - a_1 e^{-\tau} \tau \left( \int_1^z f_1(\xi) d\xi \right), \]  

\[ \Psi_s(z, \tau) = 0. \]  

(4.3.16)

### 4.3.2 Perturbation solutions on the advection (inner) timescale

In this section we will consider the system behaviour in the initial layer. We rescale time via \( \tau = \epsilon t \). We also rescale \( c_h^* \) and \( \psi_s^* \) to account for the different balances in the system in the initial layer. In particular the variables are rescaled as follows:

\[ \tau = \epsilon t, \quad C_h(z, \tau) = \frac{1}{a_1 \epsilon} c_h(z, t), \]  

(4.3.17)

\[ C_v(z, \tau) = c_v(z, t), \quad \Psi_s(z, \tau) = \frac{a_2}{a_1 \epsilon} \psi_s(z, t). \]  

(4.3.18)
The scales for each of the dimensional variables in the initial layer are
\[
\begin{align*}
  c_h^* &\sim c_{\text{sat}}, & c_v^* &\sim c_{\text{sat}}, & t^* &\sim t_a = \frac{36L^2\kappa\mu(1 - \phi_h)^2}{k_{\text{st}}\phi_h^2(\Delta P + \rho g L)}, \\
  z^* &\sim L, & \psi_s^* &\sim \psi_{s0}.
\end{align*}
\] (4.3.19, 4.3.20)

Thus the equations on the inner timescale are given by:
\[
\begin{align*}
  \frac{\partial c_h}{\partial t} &= \frac{\partial c_h}{\partial z} - \epsilon a_1(c_h - c_v) + a_2(1 - c_h)\psi_s, \\
  \frac{\partial c_v}{\partial t} &= \epsilon(c_h - c_v), \\
  \frac{\partial \psi_s}{\partial t} &= -a_2a_3(1 - c_h)\psi_s,
\end{align*}
\] (4.3.21-4.3.23)

\[
0 < z < 1, \quad t > 0,
\] (4.3.24)

\[
\begin{align*}
  c_h(z, 0) &= h(z), & c_v(z, 0) &= \eta, \\
  \psi_s(z, 0) &= 1, & c_h(1, t) &= 0.
\end{align*}
\] (4.3.25, 4.3.26)

We use the following expansions for the advection timescale:
\[
\begin{align*}
  c_h &\sim c_{h0} + \epsilon c_{h1} + \epsilon^2 c_{h2}, \\
  c_v &\sim c_{v0} + \epsilon c_{v1} + \epsilon^2 c_{v2}, \\
  \psi_s &\sim \psi_{s0} + \epsilon \psi_{s1} + \epsilon^2 \psi_{s2} \\
  h &\sim h_0 + \epsilon h_1 + \epsilon^2 h_2.
\end{align*}
\] (4.3.27-4.3.30)

### 4.3.2.1 Leading order equations

The leading order equations are:
\[
\begin{align*}
  \frac{\partial c_{h0}}{\partial t} &= \frac{\partial c_{h0}}{\partial z} + a_2(1 - c_{h0})\psi_{s0}, \\
  \frac{\partial c_{v0}}{\partial t} &= 0, \\
  \frac{\partial \psi_{s0}}{\partial t} &= -a_2a_3(1 - c_{h0})\psi_{s0}.
\end{align*}
\] (4.3.31, 4.3.32, 4.3.33)
4. COFFEE EXTRACTION IN A PACKED COFFEE BED

\[ 0 < z < 1, \quad t > 0, \quad (4.3.34) \]

\[ c_{h0}(z,0) = h_0, \quad c_{v0}(z,0) = \eta, \quad (4.3.35) \]
\[ \psi_{s0}(z,0) = 1, \quad c_{h0}(1,t) = 0. \quad (4.3.36) \]

Integrating equation (4.3.32) and applying the initial condition gives
\[ c_{v0}(z,t) = \eta. \]

Next we solve equation (4.3.33) for \( c_{h0} \) to get
\[ c_{h0} = 1 + \frac{1}{a_2 a_3 \psi_{s0}} \frac{\partial \psi_{s0}}{\partial t} \]
\[ = 1 + \frac{1}{a_2 a_3} \frac{\partial (\ln \psi_{s0})}{\partial t}. \quad (4.3.37) \]

Now substituting this into equation (4.3.31) and simplifying gives
\[ \frac{\partial^2 (\ln \psi_{s0})}{\partial t^2} = \frac{\partial^2 (\ln \psi_{s0})}{\partial t \partial z} - a_2 \frac{\partial \psi_{s0}}{\partial t}. \quad (4.3.38) \]

Integrating this with respect to time gives
\[ \frac{\partial (\ln \psi_{s0})}{\partial t} = \frac{\partial (\ln \psi_{s0})}{\partial z} - a_2 \psi_{s0} + g_1(z), \quad (4.3.39) \]

where \( g_1(z) \) is the constant of integration. Thus we have
\[ \frac{\partial \psi_{s0}}{\partial t} = \frac{\partial \psi_{s0}}{\partial z} - a_2 \psi_{s0}^2 + g_1(z) \psi_{s0}. \quad (4.3.40) \]

At \( t = 0 \) we have
\[ g_1(z) = \frac{1}{\psi_{s0}(z,0)} \left( \frac{\partial \psi_{s0}}{\partial t}(z,0) - \frac{\partial \psi_{s0}}{\partial z}(z,0) + a_2 \psi_{s0}(z,0)^2 \right). \quad (4.3.41) \]

This can be rewritten using equation (4.3.37) as
\[ g_1(z) = \frac{1}{\psi_{s0}(z,0)} \left( a_2 a_3 (c_{h0}(z,0) - 1) - \frac{\partial \psi_{s0}}{\partial z}(z,0) + a_2 \psi_{s0}(z,0)^2 \right). \quad (4.3.42) \]

Using the initial conditions \( \psi_{s0}(z,0) = 1 \) and \( c_{h0}(z,0) = h_0(z) \), we get
\[ g_1(z) = a_2 (1 + a_3 (h_0(z) - 1)). \quad (4.3.43) \]

Thus for the fine grind \( g_1(z) = a_2 \), while for the coarse grind \( g_1(z) = a_2 (1 + a_3 (\zeta(1 - z) - 1)) \). Also since \( c_{h0}(1,t) = 0 \), it is easily found that \( \psi_{s0}(1,t) = \)
exp\((-a_2a_3t)\). Thus the leading order problem for \(\psi_{s0}\) is

\[
\frac{\partial \psi_{s0}}{\partial t} = \frac{\partial \psi_{s0}}{\partial z} - a_2 \psi_{s0}^2 + g_1(z) \psi_{s0}.
\] (4.3.44)

\[
\psi_{s0}(z, 0) = 1, \quad \psi_{s0}(1, t) = e^{-a_2a_3t}.
\] (4.3.45)

We can rewrite this as

\[
\frac{\partial \psi_{s0}}{\partial t} - \frac{\partial \psi_{s0}}{\partial z} = -\psi_{s0}(g_1(z) - a_2 \psi_{s0}),
\] (4.3.46)

which we can solve using the method of characteristics. We have

\[
\frac{d\psi_{s0}}{dt} = -\psi_{s0}(g_1(z) - a_2 \psi_{s0}), \quad \text{on} \quad \frac{dz}{dt} = -1.
\] (4.3.47)

Along the characteristics \(x + t = \xi, \ \xi \) constant, we can transform the problem into

\[
\frac{d\psi_{s0}}{dt} + g_1(\xi - t) \psi_{s0} = a_2 \psi_{s0}^2.
\] (4.3.48)

This equation belongs to a general class of ordinary differential equations called Bernoulli equations. They have the form:

\[
\frac{ds}{dt} + P(t)s = Q(t)s^k,
\] (4.3.49)

where \(k \neq 0, 1\). These equations have known exact solutions. To solve, one divides the equation by \(s^k\), sets \(v(t) = s(t)^{1-k}\) and solves the resulting ODE using the integrating factor method. The process is relatively straightforward, but lengthy and will not be outlined in detail here. An exact solution in terms of \(v(t)\) is given in ref. [77] as

\[
v(t) = \exp \left( (k - 1) \int^t P(\theta)d\theta \right) \left( \int^t \exp \left( (1 - k) \int^\lambda P(\theta)d\theta \right) Q(\lambda)d\lambda \right).
\] (4.3.50)

Here the resulting solution in the specific cases of the fine and coarse grinds will be presented.
Figure 4.1: Characteristic curves $z + t = c$ of equation (4.3.46). Note solution propagates from the initial condition for $z + t < 1$, while it propagates from the boundary condition for $z + t > 1$.

**Fine grind** For the fine grind we have

$$
\frac{d\psi_{s0}}{dt} = -a_2 \psi_{s0} (1 - \psi_{s0}), \quad \text{on} \quad \frac{dz}{dt} = -1. \quad (4.3.51)
$$

If $\psi_{s0}$ is 0 or 1 it remains so, otherwise we solve the equation along the characteristics $z + t = \xi$, $\xi$ constant. The characteristics are shown in figure 4.1. In this case the equation is simpler than the general Bernoulli equation and can be solved by separation of variables. We note that the solution propagates from the initial condition at $t = 0$ for $z + t < 1$ while it propagates from the boundary condition at $z = 1$ for $z + t > 1$. In this case since the initial condition is $\psi_{s0}(z, 0) = 1$ we have $\psi_{s0} = 1$ for all $z + t < 1$. We solve equations above for $z + t > 1$ to get

$$
\psi_{s0}(z, t) = \begin{cases} 
1, & z + t < 1 \\
\frac{e^{a_2} - e^{a_2 t} + e^{a_2 (z + a_3 (z + t - 1))}}{e^{a_2} - e^{a_2 t} + e^{a_2 (z + a_3 (z + t - 1))}}, & z + t > 1.
\end{cases} \quad (4.3.52)
$$

This also gives us the leading order solution for $c_{h0}$

$$
c_{h0}(z, t) = \begin{cases} 
1, & z + t < 1 \\
\frac{e^{a_2} - e^{a_2 t} + e^{a_2 (z + a_3 (z + t - 1))}}{e^{a_2} - e^{a_2 t} + e^{a_2 (z + a_3 (z + t - 1))}}, & z + t > 1.
\end{cases} \quad (4.3.53)
$$
4.3 Asymptotic solutions

**Coarse grind**  For the coarse grind we have

\[
\frac{d\psi_{s0}}{dt} = -\psi_{s0}(a_2(1 + a_3(\zeta(1 - z) - 1)) - a_2\psi_{s0}), \quad \text{on} \quad \frac{dz}{dt} = -1. \tag{4.3.54}
\]

For \(0 < z + t = \xi < 1\) we solve

\[
\frac{d\psi_{s0}}{dt} = -\psi_{s0}(a_2(1 + a_3(\zeta(1 + t - \xi) - 1)) - a_2\psi_{s0}), \tag{4.3.55}
\]

\[
\psi_{s0}(\xi) = 1. \tag{4.3.56}
\]

The solution for \(z + t < 1\) is given by

\[
\psi_{s0}(z, t) = \frac{n_1(z, t)}{n_2(z, t)}, \tag{4.3.57}
\]

where

\[
n_1(z, t) = 2\sqrt{a_3}\exp\left(\frac{a_2(a_3^2(2t + z^2 + 1)))}{2a_3}\right) \tag{4.3.58}
\]

\[
+ 2\sqrt{a_3}\exp\left(\frac{a_2(a_3(2\zeta(az + t + 1) + a_3) + 1)}{2a_3}\right) \tag{4.3.59}
\]

and

\[
n_2(z, t) = \sqrt{2\pi a_2 e^{\frac{a_3^2(1)((t+z)+1)}{\zeta}}} \left(\text{erfi}\left(\frac{a_3\zeta(t + z - 1) + a_3 - 1}{\sqrt{2} \sqrt{\frac{a_3^2}{a_2}}}ight)\right) \tag{4.3.60}
\]

\[
- \sqrt{2\pi a_2 e^{\frac{a_3^2(1)((t+z)+1)}{\zeta}}} \left(\text{erfi}\left(\frac{a_3\zeta(z - 1) + a_3 - 1}{\sqrt{2} \sqrt{\frac{a_3^2}{a_2}}}ight)\right) \tag{4.3.61}
\]

\[
+ 2\sqrt{a_3}\exp\left(\frac{1}{2} a_2 \left( a_3\zeta + \frac{a_3}{\zeta} + \frac{1}{a_3\zeta} + a_3\zeta(t + z)^2 + 2a_3(t + z) + 2 \right)\right). \tag{4.3.62}
\]

The solution for \(c_{h0}\) is then got using equation (4.3.37). For \(z + t = \xi > 1\) we solve

\[
\frac{d\psi_{s0}}{dt} = -\psi_{s0}(a_2(1 + a_3(\zeta(1 + t - \xi) - 1)) - a_2\psi_{s0}), \tag{4.3.63}
\]

\[
\psi_{s0}(\xi) = e^{-a_2a_3(\xi-1)}. \tag{4.3.64}
\]
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The solution for $z + t > 1$ is given by

$$\psi_{s0}(z, t) = \frac{n_3(z, t)}{n_4(z, t)}, \quad (4.3.63)$$

where

$$n_3(z, t) = 2\sqrt{a_3} \exp \left( \frac{a_2 ((a_3\zeta(z - 1) + a_3)^2 - 2a_3\zeta(z - 1) + 1)}{2a_3} \right), \quad (4.3.64)$$

and

$$n_4(z, t) = 2\sqrt{a_3} \exp \left( \frac{a_2 (a_3^2 + 1) + a_2a_3(t+z-1)}{2a_3} \right) + \sqrt{2\pi} \sqrt{a_2} e^{a_2/\zeta} \left( \frac{a_3 - 1}{\sqrt{2} a_2} \right) \left( \text{erfi} \left( \frac{a_3\zeta(z - 1) + a_3 - 1}{\sqrt{2} a_2} \right) \right) - \sqrt{2\pi} \sqrt{a_2} e^{a_2/\zeta} \left( \frac{a_3\zeta(z - 1) + a_3 - 1}{\sqrt{2} a_2} \right) \left( \text{erfi} \left( \frac{a_3\zeta(z - 1) + a_3 - 1}{\sqrt{2} a_2} \right) \right). \quad (4.3.65)$$

The solution for $c_{h0}$ is then got using equation (4.3.37).

These solutions are given in terms of the imaginary error function defined by

$$\text{erfi}(z) = \frac{1}{i} \text{erf}(iz) = \frac{2}{\sqrt{\pi} \sqrt{i} \int_0^{iz} e^{-t^2} dt}. \quad (4.3.66)$$

4.3.2.2 Order $\epsilon$ equations

The order $\epsilon$ equations are

$$\frac{\partial c_{h1}}{\partial t} = \frac{\partial c_{h1}}{\partial z} + a_2(1 - c_{h0})\psi_{s1} - a_1(c_{h0} - c_{v0}) - a_2c_{h1}\psi_{s0}, \quad (4.3.67)$$

$$\frac{\partial c_{v1}}{\partial t} = c_{h0} - c_{v0}, \quad (4.3.68)$$

$$\frac{\partial \psi_{s1}}{\partial t} = -a_2a_3(1 - c_{h0})\psi_{s1} + a_2a_3c_{h1}\psi_{s0}, \quad (4.3.69)$$

$$0 < z < 1, \quad t > 0, \quad (4.3.70)$$
4.3 Asymptotic solutions

\[ c_{h1}(z,0) = h_1(z), \quad c_{v1}(z,0) = 0, \quad (4.3.71) \]
\[ \psi_{s1}(z,0) = 0, \quad c_{h1}(1,t) = 0. \quad (4.3.72) \]

Note for both the fine and coarse grinds we have \( h_1(z) = 0 \). First we solve (4.3.68). We substitute the known values in for \( c_{h0} \) and \( c_{v0} \). The solution for the coarse grind in the initial layer isn’t possible beyond leading order. We proceed here with the solution for the fine grind. As \( c_{h0} \) is different for \( z + t < 1 \) and \( z + t > 1 \) so is \( c_{v1} \). Solving the equations we find

\[ c_{v1}(z,t) = \begin{cases} (1 - \eta)t + \frac{1}{a_2a_3} \ln \left( \frac{e^{a_2} - e^{a_2z} + e^{a_2(z+t)}(z+t-1)}{e^{a_2z}+1} \right), & z + t < 1 \\ (1 - \eta)t + 1, & z + t > 1 \end{cases} \quad (4.3.73) \]

Next we solve (4.3.69) for \( c_{h1} \) in terms of \( \psi_{s1} \). We can do this for \( z + t < 1 \) and \( z + t > 1 \) but only the former yields a solution for \( \psi_{s1} \) and \( c_{h1} \) and so only this is presented here. For \( z + t < 1 \) we get

\[ c_{h1} = \frac{1}{a_2a_3} \frac{\partial \psi_{s1}}{\partial t}. \quad (4.3.74) \]

As was done at leading order, we can substitute this into (4.3.67), integrate with respect to time and use initial conditions to evaluate constant of integration. This leads to the equation

\[ \frac{\partial \psi_{s1}}{\partial t} - \frac{\partial \psi_{s1}}{\partial z} = -a_2\psi_{s1} - \eta a_1a_2a_3t. \quad (4.3.75) \]

Again this can be solved by the method of characteristics so that for \( z + t < 1 \) we have

\[ \psi_{s1}(z,t) = \frac{a_1a_3((\eta - 1)e^{-a_2t}(1 + e^{a_2t}(a_2t - 1)))}{a_2}. \quad (4.3.76) \]

This also gives us \( c_{h1} \) for \( z + t < 1 \)

\[ c_{h1}(z,t) = \frac{a_1(\eta - 1)e^{-a_2t}(e^{a_2t} - 1)}{a_2}. \quad (4.3.77) \]

The same steps can be tried for \( z + t > 1 \), however the integration with respect to time is not possible in this case.
4. COFFEE EXTRACTION IN A PACKED COFFEE BED

4.3.2.3 Solutions on the advection (inner) timescale

In summary for the fine grind we have the following inner solutions:

\[ c_h(z,t) = \begin{cases} 
1 + \epsilon \left( \frac{a_1(\eta-1)e^{-a_2(1+e^{a_2(t-1)})}}{e^{a_2-a_2^2+z+a_3(t+z-1)}} \right), & z + t < 1 \\
\frac{e^{a_2-a_2^2+z+a_3(t+z-1)}}{e^{a_2-a_2^2+z+a_3(t+z-1)}} & z + t > 1, 
\end{cases} \quad (4.3.78) \]

\[ c_v(z,t) = \begin{cases} 
\eta + \epsilon \left( (1-\eta)t + \frac{1}{a_2 a_3} \ln \left( \frac{e^{a_2-a_2^2+z+a_3(t+z-1)}}{e^{a_2-a_2^2+z+a_3(t+z-1)}} \right) \right), & z + t < 1 \\
\frac{e^{a_2-a_2^2+z+a_3(t+z-1)}}{e^{a_2-a_2^2+z+a_3(t+z-1)}} & z + t > 1, 
\end{cases} \quad (4.3.79) \]

\[ \psi_s(z,t) = \begin{cases} 
1 + \epsilon \left( \frac{a_1 a_3 (\eta-1) e^{-a_2 (1+e^{a_2(t-1)})}}{e^{a_2-a_2^2+z+a_3(t+z-1)}} \right), & z + t < 1 \\
\frac{e^{a_2-a_2^2+z+a_3(t+z-1)}}{e^{a_2-a_2^2+z+a_3(t+z-1)}} & z + t > 1. 
\end{cases} \quad (4.3.80) \]

The solutions for the coarse grinds are known at leading order but are prohibitively untidy to reproduce here.

4.3.3 Matching

We can find the constants of integration remaining in the outer solution by using modified Van Dyke matching [71] to match the initial layer solution with the outer solution. This method involves comparing the inner expansion of the outer solutions with the outer expansion of the inner (initial layer) solutions to obtain unknown functions \( f_1(z) \) and \( f_2(z) \) in equations (4.3.14) and (4.3.15).

**Fine grind** For the fine grind initial conditions this yields:

\[ f_1(z) = \eta, \quad f_2(z) = \left( \frac{1}{a_3} + 1 \right) (1 - z). \quad (4.3.81) \]
Thus the outer solutions are:

\[ C_h(z, \tau) = e^{-\tau}(\eta - \eta z) \]
\[ + \epsilon \left( \frac{1}{2a_3} e^{-\tau} ((z - 1)^2 (1 + a_3(1 + \eta(1 + a_1(\tau - 1)))) \right), \]
\[ C_v(z, \tau) = \eta e^{-\tau} \]
\[ + \epsilon \left( -e^{-\tau}(-\eta a_1 + \eta a_1 z) \tau + e^{-\tau} \left( \frac{1}{a_3} + 1 \right) (1 - z) \right), \]
\[ \Psi_s(z, \tau) = 0. \]

Coarse grind For the coarse grind initial conditions this yields:

\[ f_1(z) = \eta, \quad f_2(z) = 0. \]

Thus the outer solutions are:

\[ C_h(z, \tau) = e^{-\tau}(\eta - \eta z) \]
\[ + \epsilon \left( \frac{1}{2} \eta e^{-\tau}(z - 1)^2 (a_1(\tau - 1) + 1) \right), \]
\[ C_v(z, \tau) = \eta e^{-\tau} + \epsilon \left( e^{-\tau} \eta a_1 (1 - z) \right), \]
\[ \Psi_s(z, \tau) = 0. \]

4.3.4 Composite solutions

Fine grind We have inner and outer solutions for our equations. For \( c_h \) we obtain an expansion to leading order in the inner layer and to \( O(\epsilon) \) in the outer region. The solution for \( c_v \) is known to \( O(\epsilon) \) in both regions while \( \psi_s \) has an inner solution at leading order while the outer solution is 0 to \( O(\epsilon) \). Comparison with numerics show that the inner and outer solutions fit quite well in their regions of validity. In terms of the initial layer scalings the outer solution for \( c_h \) is zero at leading order. As the initial layer solution can only be determined at leading order the inner and outer solutions for \( c_h \) have no common part. Thus the composite solution is just their sum. The solution for \( c_v \) was formed by matching so we can easily identify the common part and subtract it off. The composite solution for \( \psi_s \) is just the inner solution. In terms of the inner scalings and the Heaviside or unit step function \( \mathcal{H}(x) \), the composite solutions are
4. COFFEE EXTRACTION IN A PACKED COFFEE BED

\[ c_h(z, t) = \left( 1 + \epsilon \left( \frac{a_1 e^{-\alpha t} (\eta - 1) (e^{\alpha t} - 1)}{a_2} \right) \right) \mathcal{H}(1 - (z + t)) \]
\[ + \left( \frac{e^{a_2} - e^{a_2 z}}{e^{a_2 z} + e^{a_2 (z + t + 1)}} \right) \mathcal{H}((z + t) - 1) \]
\[ + \epsilon a_1 \left( e^{-\epsilon t} (\eta - \eta z) + \epsilon \left( \frac{1}{2a_3} e^{-\epsilon t} \left( (z - 1)^2 (1 + a_3 (1 + a_4 (\epsilon t - 1))) \right) \right) \right), \]

(4.3.89)

\[ c_v(z, t) = (\eta + \epsilon ((1 - \eta) t)) \mathcal{H}(1 - (z + t)) \]
\[ + \left( \eta + \epsilon \left( (1 - \eta) t + \frac{1}{a_2 a_3} \ln \left( e^{a_2} - e^{a_2 z} + e^{a_2 (z + t + 1)} \right) \right) \right) \mathcal{H}((z + t) - 1) \]
\[ \eta e^{-\epsilon t} + \epsilon \left( -e^{-\epsilon t} (-\eta a_1 + \eta a_1 z) \epsilon t + e^{-\epsilon t} \left( \frac{1}{a_3} + 1 \right) (1 - z) \right) \]
\[ - (\eta - \eta \epsilon t + \epsilon \left( \frac{1}{a_3} + 1 \right) (1 - z)), \]

(4.3.90)

\[ \psi_s(z, t) = \left( 1 + \epsilon \left( a_1 a_3 ((\eta - 1) e^{-\alpha t} (1 + e^{\alpha t} (a_2 t - 1))) \right) \right) \mathcal{H}(1 - (z + t)) \]
\[ + \left( \frac{e^{a_2}}{e^{a_2} - e^{a_2 z} + e^{a_2 (z + t + 1)}} \right) \mathcal{H}((z + t) - 1), \]

(4.3.91)

where \( \mathcal{H}(x) \) is defined by

\[ \mathcal{H}(x) = \begin{cases} 
1 & \text{if } x \geq 0, \\
0 & \text{if } x < 0. 
\end{cases} \]

Coarse grind  We have inner and outer solutions for our equations. For \( c_h \) and \( c_v \) we obtain an expansion to leading order in the inner layer and to \( O(\epsilon) \) in the outer region. For \( \psi_s \) we have an inner solution at leading order while the outer solution is \( 0 \) to \( O(\epsilon) \). Comparison with numerics show that the inner and outer solutions fit quite well in their regions of validity. In terms of the initial layer scalings the outer solution for \( c_h \) is zero at leading order. As the initial layer solution can only be determined at leading order the inner and outer solutions for \( c_h \) have no common part. Thus the composite solution is just their sum. The
solution for $c_v$ was formed by matching so we can easily identify the common part and subtract it off. The composite solution for $\psi_s$ is just the inner solution. We denote the initial layer solutions found at leading order for $c_h$ as $c_{ha}$ for $z + t < 1$ and $c_{hb}$ for $z + t > 1$ and for $\psi_s$ as $\psi_{sa}$ for $z + t < 1$ and $\psi_{sb}$ for $z + t > 1$. In terms of the inner scalings and the Heaviside or unit step function $\mathcal{H}(x)$, the composite solutions are

$$c_h(z, t) = c_{ha}(z, t)\mathcal{H}(1 - (z + t)) + c_{hb}(z, t)\mathcal{H}((z + t) - 1) - \eta e^{-\epsilon t}(z - 1) + \epsilon \left( \frac{1}{2}\eta e^{-\epsilon t}(z - 1)^2(a_1(\epsilon t - 1) + 1) \right), \quad (4.3.93)$$

$$c_v(z, t) = \eta e^{-\epsilon t} + \epsilon \left( e^{-\epsilon t}(a_1\eta - a_1\eta z) \right), \quad (4.3.94)$$

$$\psi_s(z, t) = \psi_{sa}(z, t)\mathcal{H}(1 - (z + t)) + \psi_{sb}(z, t)\mathcal{H}((z + t) - 1). \quad (4.3.95)$$

### 4.3.5 Comparison of asymptotics with numerical simulation

Equations (4.3.21) - (4.3.26) are solved numerically using the numerical method of lines and compared to the derived composite solutions. The parameters used are those corresponding to JK drip filter grind and Cimbali # 20 drip filter grind.

**Fine grind** The plots for the JK drip filter grind parameters are shown in figures [4.2](#) - [4.7](#). Figure 4.2 plots the concentration through the bed at different times. At leading order the inner and outer solutions for $c_h$ match identically. As the inner solution could only be determined at leading order and the outer solution is zero at this order, the common part is zero. For this reason the composite solution does not agree well with numerical solution initially, although inner and outer solutions agree well with the numerical solution over their regions of validity. Figure 4.3 plots the concentration at the filter exit ($z = 0$) against time. Data points from experiment (in non-dimensional units) are also included for comparison. The inner and outer solutions are plotted separately in the second plot to illustrate their agreement with the numerical solution. The agreement
with experimental data shows that the reduced system of equations can still reproduce the experimentally determined extraction profile. Figures 4.4-4.7 include the corresponding plots for \( c_v \) and \( \psi_s \). Asymptotic solutions are only compared to numerical solutions in this case, due to difficulties in obtaining experimental data for \( c_v \) and \( \psi_s \). As was the case with \( c_h \), the disagreement between the asymptotic and numerical solutions for short times with \( z + t > 1 \) is due to the absence of an order \( \epsilon \) term in this solution.

**Figure 4.2:** Plot of numerical (- -) and composite (–) solutions with \( \epsilon = 0.127 \), \( a_1 = 2.81 \), \( a_2 = 5.139 \), \( a_3 = 0.473 \), \( \eta = 0.5 \) (JK drip filter grind) of \( c_h \) vs. \( z \) at \( t = 0 \), \( t = 0.5 \), \( t = 1 \), \( t = 2 \) and \( t = 5 \).

**Coarse grind** The plots for the Cimbali #20 grind parameters are shown in figures 4.8-4.13. Figure 4.8 plots the concentration through the bed at different times. Again at leading order the inner and outer solutions for \( c_h \) match identically. The initial layer solution is only known at leading order so as expected the error is of \( O(\epsilon) \). Figure 4.9 plots the concentration at the filter exit (\( z = 0 \)) against time. Data points from experiment (in non-dimensional units) are also included for comparison. The inner and outer solutions are plotted separately in the second plot to illustrate their agreement with the numerical solution. The agreement with experimental data shows that the reduced system of equations can still reproduce the experimentally determined extraction profile, although there is some disagreement initially which suggests different fitting parameters than in chapter 2 should be used. Figures 4.10-4.13 include the corresponding
4.3 Asymptotic solutions

![Figure 4.3](image_url)

**Figure 4.3:** Plot of numerical (---) and composite (--) solutions with $\epsilon = 0.127$, $a_1 = 2.81$, $a_2 = 5.139$, $a_3 = 0.473$, $\eta = 0.5$ (JK drip filter grind) of (a)$c_h$ vs. $t$ at $z = 0$. Experimental data points are included. (b)Plot of numerical solution (---) and inner (- -) and outer (--) solutions of $c_h$ vs. $t$ at $z = 0$. Experimental data points are included.

![Figure 4.4](image_url)

**Figure 4.4:** Plot of numerical (--) and composite (--) solutions with $\epsilon = 0.127$, $a_1 = 2.81$, $a_2 = 5.139$, $a_3 = 0.473$, $\eta = 0.5$ (JK drip filter grind) of $c_v$ vs. $z$ at $t = 0$, $t = 2$, $t = 6$, $t = 15$ and $t = 30$.

As was the case with $c_h$, the disagreement between the asymptotic and numerical solutions for short times with $z + t > 1$ is due to the absence of an order $\epsilon$ term in this solution. Non-uniform extraction of $c_v$ for $z + t < 1$ is not picked up at leading order so the error is larger at the filter exit.
Figure 4.5: Plot of numerical (--) and composite (--) solutions with $\epsilon = 0.127$, $a_1 = 2.81$, $a_2 = 5.139$, $a_3 = 0.473$, $\eta = 0.5$ (JK drip filter grind) of (a)$c_v$ vs. $t$ at $z = 0$, (b) Plot of numerical (--) and inner (- -) and outer (--) solutions of $c_v$ vs. $t$ at $z = 0$.

Figure 4.6: Plot of numerical (--) and composite (--) solutions solutions with $\epsilon = 0.127$, $a_1 = 2.81$, $a_2 = 5.139$, $a_3 = 0.473$, $\eta = 0.5$ (JK drip filter grind) of $\psi_s$ vs. $z$ at $t = 0$, $t = 0.5$, $t = 1$, $t = 2$ and $t = 3$.

4.4 Conclusion

In this chapter we consider some approximate solutions to the coffee extraction model described in chapter 2. The model equations are simplified and non-dimensionalised to describe extraction from a packed coffee bed. Approximate solutions for extraction from a dilute suspension of coffee grains is considered in chapter 3. The non-dimensional equations depend on a small number of param-
4.4 Conclusion

Figures 4.7: Plot of numerical (—) and composite (–) solutions with $\epsilon = 0.127$, $a_1 = 2.81$, $a_2 = 5.139$, $a_3 = 0.473$, $\eta = 0.5$ (JK drip filter grind) of $\psi_s$ vs. $t$ at $z = 0$.

Figures 4.8: Plot of numerical (—) and composite (–) solutions with $\epsilon = 0.036$, $a_1 = 2.0461$, $a_2 = 0.866$, $a_3 = 0.84$, $\zeta = 0.4$, $\eta = 0.5$ (Cimbali #20 grind) of $c_h$ vs. $z$ at $t = 0$, $t = 0.5$, $t = 1$, $t = 2$ and $t = 5$.

Parameters and represent a vast simplification of the original equations. We can form approximate solutions to these equations using perturbation techniques. The non-dimensional parameters are directly related to the physical parameters of extraction, so these solutions are useful to investigate how a particular parameter affects the extraction profile.

Approximate solutions are formed for the model equations which describe coffee extraction from a packed bed by a pressure driven flow of hot water. The solutions are based on the presence of a small parameter in the system. The small parameter used is the ratio of the advective timescale to the grain diffusion
Figure 4.9: Plot of numerical (– –) and composite (–) solutions with $\epsilon = 0.036$, $a_1 = 2.0461$, $a_2 = 0.866$, $a_3 = 0.84$, $\zeta = 0.4$, $\eta = 0.5$ (Cimbali #20 grind) of (a)$c_h$ vs. $t$ at $z = 0$. Experimental data points are included. (b)Plot of numerical solution (– –) and inner (- -) and outer (–) solutions of $c_h$ vs. $t$ at $z = 0$. Experimental data points are included.

Figure 4.10: Plot of numerical (– -) and composite (–) solutions with $\epsilon = 0.036$, $a_1 = 2.0461$, $a_2 = 0.866$, $a_3 = 0.84$, $\zeta = 0.4$, $\eta = 0.5$ (Cimbali #20 grind) of $c_v$ vs. $z$ at $t = 0$, $t = 2$, $t = 6$, $t = 15$ and $t = 30$. timescale. The initial conditions also need to be estimated here. Different initial conditions are prescribed depending on whether a coarse or fine coffee grind is used, thus leading to different approximate solutions in these situations. It is possible to find solutions for initial conditions which define the initial concentration in the bed as a function of bed depth. Solutions are presented here for a constant initial concentration in the intergranular pores at coffee solubility and a
4.4 Conclusion

Figure 4.11: Plot of numerical (--) and composite (-) solutions with $\epsilon = 0.036$, $a_1 = 2.0461$, $a_2 = 0.866$, $a_3 = 0.84$, $\zeta = 0.4$, $\eta = 0.5$ (Cimbali #20 grind) of (a)$c_v$ vs. $t$ at $z = 0$, (b) Plot of numerical (--) and inner (-) and outer (-) solutions of $c_v$ vs. $t$ at $z = 0$.

Figure 4.12: Plot of numerical (--) and composite (-) solutions with $\epsilon = 0.036$, $a_1 = 2.0461$, $a_2 = 0.866$, $a_3 = 0.84$, $\zeta = 0.4$, $\eta = 0.5$ (Cimbali #20 grind) of $\psi_s$ vs. $z$ at $t = 0$, $t = 0.5$, $t = 1$, $t = 2$ and $t = 3$.

concentration which is linear with bed depth. Approximate solutions are formed and compared to the numerical solution of the equations and the available experimental data. These solutions allow the coffee quality (in terms of brew strength and extraction yield) at a given time to be explicitly written in terms of the process parameters of the system by integrating the exiting concentration. This can be done as in section 2.7. Such solutions have potential to be used to evaluate a particular brewing set-up or investigate the impact of changing certain brewing
4. COFFEE EXTRACTION IN A PACKED COFFEE BED

Figure 4.13: Plot of numerical (—) and composite (—) solutions with $\epsilon = 0.036$, $a_1 = 2.0461$, $a_2 = 0.866$, $a_3 = 0.84$, $\zeta = 0.4$, $\eta = 0.5$ (Cimbali #20 grind) of $\psi_s$ vs. $t$ at $z = 0$. 

parameters.
CHAPTER 5

INfiltration into a dry coffee bed

5.1 Introduction

In the previous chapters, we considered extraction from a doubly porous packed coffee bed. The assumption was made that the coffee brewing process in this situation can be broken into three stages:

1. Initially, in the filling stage, hot water infiltrates into the dry coffee bed under the influence of an applied pressure. It is assumed that no water exits the bed, until a volume of water sufficient to fill all the pore volume (intergranular and intragranular) has flowed into the bed.

2. Once this has occurred, the bed is saturated with liquid and liquid starts to exit from the bed. We refer to this next stage as the steady state stage, as it is assumed that there is a steady flow of liquid through the bed, with liquid entering and leaving the bed at the same rate.

3. Finally the draining stage occurs, when water delivery to the bed is shut off and interstitial liquid between the grains drains from the bed.

This conceptual model of extraction as three discrete stages is of course a simplification of reality, only justified if the key mechanisms of extraction can be
5. INFILTRATION INTO A DRY COFFEE BED

captured. It does however offer some advantages. The steady state stage encompasses most of the brewing time, and, under the assumption of a fluid saturated bed during this time, is the simplest to model. Modelling carried out on this stage, shows that the coffee extraction profiles from the bed can be fitted to experiments, without modelling unsaturated flow during filling and draining periods, provided sensible initial conditions are chosen for the coffee concentrations in the bed following the filling stage. Care needs to be taken that the total amount of coffee solubles in the bed following filling (in solution and or still undissolved), is the same is the amount of coffee solubles (undissolved) in dry coffee. This just places a constraint on the initial conditions that can be chosen. The drainage stage is not important for extraction since most of the coffee solubles have been extracted at this stage and the extraction rate is slow. It is important that the correct volume of fluid is delivered to the coffee pot, to determine the final coffee beverage strength, if this is a priority. To this end, care should be taken to allow for the retention of residual fluid which does not drain from the bed.

It is clear that we can model extraction, just considering the steady state stage, by carefully choosing initial concentrations following the filling stage. However this is a little unsatisfactory and clearly it is desirable to extend our model to include unsaturated flow during the filling stage. While this is quite possible in theory, there are a number of extra processes occurring during the filling stage which complicate the situation. Some of these processes are poorly understood, and where models do exist, their relative influence on the infiltration dynamics is not known. Furthermore there is little or no experimental data or insight to base a theory on. So, while it is possible to formulate multiple models based on different physical mechanisms, it is impossible to parametrise or validate the models without some experimental insight and data. Thus the aims of this section are:

1. Discuss the complications of modelling the filling stage.

2. Outline some general models of infiltration.

3. Apply a simplified model, to provide an initial estimate of coffee concentration profiles in the packed coffee bed after the filling stage, for the experiments with fine and coarse coffee grinds.
5.2 Infiltration of hot water into a packed coffee bed under the influence of an applied pressure

In the situation of interest here, ground coffee is placed in a cylindrical brewing chamber, resting on a filter supported by a stainless steel mesh. The bed is lightly compacted and a stainless steel mesh is placed above the bed, mainly to ensure an even flow of water the bed. The bed is connected to a rotary vane pump which can supply water to the bed at pressures of up to 15 bar. When there is no resistance to flow, the pump operates at its maximum possible flow rate for a given pressure, governed by the pump’s pressure-flow characteristic. When resistance is added (e.g. the coffee bed) the applied pressure stays the same but the flow rate adjusts to the new resistance.

During infiltration there are several physical processes occurring. Initially at time $t = 0$, the pump is switched on at a given applied pressure $\Delta P$. Immediately before the water comes in contact with the bed, the pump is operating at its maximum flow rate for the particular applied pressure. As soon as the water hits the grind, considerable momentum is transferred to the grind, leading to compaction of the coffee bed. Water infiltrating into the bed meets considerable resistance as it flows over and between grain surfaces. Coupled with this, water may be infiltrating into the fibrous cellular grain structure causing grain swelling. Thus, with ongoing water penetration and grain swelling, the counter pressure of the bed increases, sharply reducing the flow rate. In experiments performed with shallow coffee beds, all these processes seem to occur in the first 5 seconds. The volume of water delivered in this time is probably sufficient to saturate the coffee bed. At $t^* = 5–10$ seconds the flow rate is observed to reach a minimum before rising, to a limited extent, to what appears to be an equilibrium value after this. It is not clear exactly how this behaviour changes for beds with a greater depth and longer infiltration time. The equilibrium flow rate is determined by the applied pressure and resistance provided by the compressed coffee bed. Measurement of the equilibrium flow rate allows the equilibrium bed porosity to be estimated from the Kozeny-Carman equation. This equilibrium flow rate corresponds to what we have called the steady state stage above.
5. INFILTRATION INTO A DRY COFFEE BED

The reason why the flow rate reaches a minimum before gradually increasing again is unclear. This may be related to extraction (which may open up some extra space for water passage) and/or to the rearrangement of fine cell fragments in the coffee bed to open up some preferential flow paths. It is clear that the dynamics of infiltration depend, to a greater or lesser extent, on a number of mechanisms including bed compaction, grain swelling, coffee extraction and air trapping. Another potential complication arises from the presence of trapped gas (87% carbon dioxide and 13% volatile aromatics) \[57\], in the coffee grain matrix. These gases are trapped in closed coffee cells under pressure during roasting. Levels of these gases are highest in freshly ground coffee. Wetting and swelling of the grains causes the release of these gases. As carbon dioxide is not very soluble in hot water, this degassing may have an influence on the flow through the bed. The relative influence of these processes on infiltration would require extensive experimental investigation to determine.

5.3 Literature review: Infiltration of a liquid into a porous medium

The general problem of infiltration of a liquid into a porous medium has been widely studied. Hydrologists, in particular, have studied the infiltration of water (rainfall) into soils and infiltration of water into aquifers from water storage ponds and lakes. This subject and more generally the subject of movement of water into and through the vadose zone (unsaturated zone) in soils is “of great importance to the assessment of contaminant fate and transport, agricultural management and natural resource protection” \[73\]. Models of infiltration vary from purely empirical equations, with a small number of fitting parameters, to mechanistic models based on a simplified representation of the physical mechanisms of infiltration, to models which try to model flow of both air and water in the unsaturated porous medium during infiltration. Simple empirical models are, of course, easy to apply given some basic experimental data to parametrise them, but suffer from a lack of detail and adaptability to changes in the porous media structure (without new experimental data). Complex models which attempt to describe infiltration in terms of the various physical characteristics of the porous medium, are much more adaptable (provided they capture the physical mechanisms correctly), but
are based on knowledge of the hydraulic properties of the porous medium in question, which must be determined from experiment. Striking a balance between a model which is sufficiently rich to capture the important mechanisms of infiltration, but is simple enough to parametrise and solve, is a difficult task. In this section, to motivate later developments, some of the basic models of infiltration which have been applied to model soil physics will be outlined.

### 5.3.1 Darcy’s law

Many of the developments in the study of flow in unsaturated porous media have occurred in the last century, but the first important contribution, a century earlier, related to saturated flow. Models governing water flow in saturated porous media are largely based on the work of French engineer Henry Darcy. In 1856 Darcy formulated the first empirical quantitative description of flow through a saturated porous medium, based on his observations from experiments on water filtration through sand beds [4]. Darcy summarised his findings for flow through a vertical, saturated, homogenous sand filter in his famous equation, now known as Darcy’s law:

\[
q = \frac{Q}{A} = -K_s \frac{\Delta h}{L} = -K_s \frac{h_2 - h_1}{L},
\]

where \( Q \) is the rate of flow into the column, \( A \) is the column flow rate, \( q \) is the specific discharge or Darcy flux (velocity), \( L \) is the column length and \( \Delta h \) is the difference between the hydraulic heads at the column outlet \( h_2 \) and the column inlet \( h_1 \). Darcy’s law says that the rate of flow through the column, is proportional to the column cross-sectional area and the difference in hydraulic heads, but inversely proportional to the column length. The constant of proportionality is given by the (saturated) hydraulic conductivity \( K_s \). More generally, the one dimensional version of Darcy’s law for a flow in the \( z \)-direction is given by:

\[
q = -K_s \frac{\partial h}{\partial z},
\]

where \( \frac{\partial h}{\partial z} \) is the hydraulic gradient. The hydraulic head is usually broken up into a pressure head and an elevation head:

\[
h = \psi + z,
\]

where \( \psi \) is the pressure head.
where $\psi = \frac{p}{\rho g}$ and $z$ is the elevation above the datum. Here $p$ is the pressure in the fluid, $\rho$ is the fluid density and $g$ is acceleration due to gravity. This means Darcy’s law can be restated in the following forms

$$q = -K_s \left( \frac{\partial \psi}{\partial z} + 1 \right), \quad q = -\frac{k}{\mu} \left( \frac{\partial p}{\partial z} + \rho g \right),$$

(5.3.4)

where $k = \frac{K_s \mu}{\rho g}$ is the permeability and $\mu$ is the fluid viscosity.

### 5.3.2 The Buckingham-Darcy law

In 1907 Buckingham extended Darcy’s law to model unsaturated flows, where the volumetric water content $\theta$ is less than its maximum value $\theta_s$, which corresponds to full saturation. Buckingham’s main assumption was that the saturated hydraulic conductivity $K_s$ could be replaced by a function of the soil volumetric water content $\theta$, or the (capillary) pressure head $\psi$. Thus $K_s$ in Darcy’s law can be replaced by $K(\theta)$ or $K(\psi)$. This also suggests that we can relate $\psi$ and $\theta$, say through a relationship of the form $\psi = f(\theta)$. This relationship is commonly referred to as the water retention curve or soil moisture characteristic [60]. If the air forms a continuous phase, the hydrostatic pressure in the water ($p_w$) is less than the pressure in the air ($p_a$). Thus, if the air is assumed to be at atmospheric pressure, the gauge pressure, $p = p_w - p_a$, is negative. The capillary pressure is defined as $p_c = p_a - p_w$, the pressure in the non-wetting phase (air) minus the pressure in the wetting phase (water). Thus

$$\psi = \frac{p}{\rho g} = -\frac{p_c}{\rho g},$$

(5.3.5)

is negative in the unsaturated porous medium. It should be noted that sometimes $\psi$ is defined with the opposite sign and used to denote capillary suction. The Buckingham-Darcy law in a porous medium is now given by

$$q = -K(\psi) \left( \frac{\partial \psi}{\partial z} + 1 \right) = -K(\theta) \left( \frac{\partial \psi(\theta)}{\partial z} + 1 \right).$$

(5.3.6)

### 5.3.3 The Richards’ equation

In 1931 Richards combined the Buckingham-Darcy law with the principle of continuity (conservation of mass of water), to form a general equation for flow through
a porous medium. The general equation of continuity is
\[ \frac{\partial \theta \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{q}). \tag{5.3.7} \]

For one-dimensional infiltration in the \( z \)-direction, with constant water density, this reduces to
\[ \frac{\partial \theta}{\partial t} + \frac{\partial q}{\partial z} = 0. \tag{5.3.8} \]

Now we can substitute in for \( q \) to obtain the famous Richards’ equation:
\[ \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left( K(\psi) \left( \frac{\partial \psi}{\partial z} + 1 \right) \right). \tag{5.3.9} \]

Richards’ equation can be presented in various forms. The above formulation is referred to as the mixed form. The other two main formulations are the pressure head formulation and the saturation based formulation. The pressure head formulation is
\[ C(\psi) \frac{\partial \psi}{\partial t} = \frac{\partial}{\partial z} \left( K(\psi) \left( \frac{\partial \psi}{\partial z} + 1 \right) \right), \tag{5.3.10} \]
where \( C(\psi) = \frac{d\theta}{d\psi} \) is defined as the specific moisture capacity function.

The saturation based formulation is
\[ \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left( D(\theta) \frac{\partial \theta}{\partial z} + K(\theta) \right), \tag{5.3.11} \]
where \( D(\theta) = K(\theta) \frac{d\psi}{d\theta} = \frac{K(\theta)}{C(\theta)} \) is the soil water diffusivity. The equation can also be written in terms of \( p \) by substituting \( \psi = \frac{p}{\rho g} \). The choice of representation of the Richards’ equation depends on the problem to be solved and the parametric functions available to relate the variables \( \psi \), \( \theta \) and \( K \). Analytic solutions to Richards’ equation can only be derived for specific sets of initial and boundary conditions and hydraulic properties and it must generally be solved numerically. The hydraulic properties of a porous medium must be established by experiment. A host of mathematical relationships have been suggested in the literature to relate the hydraulic conductivity, pressure head and water content. Some of these are summarised in ref. [65]. These relationships contain fitting parameters which must be fitted to experimental data. Richards’ equation is limited to situations with constant density \( \rho \) and where the air phase is arbitrarily mobile, such that the pressure gradient required to move it is negligible in comparison to the
pressure gradient required to move the water phase \[59\]. These limitations mean
that more complicated and complete models have been developed. In particu-
lar, whenever air flow is important in the infiltration dynamics, the movement
of air in the porous medium should be modelled as well, using two-phase flow
equations. Air entrapment and counterflow can occur in certain situations, dra-
matically reducing the infiltration. For example, a recent paper \[67\] conducted
experiments comparing infiltration into an initially dry vertical porous medium
under unconfined (air is free to exit porous medium at the outlet) and confined
(air cannot exit porous medium at the outlet) conditions. The pressure build-
up and counterflow of air in the confined case was found to dramatically reduce
the infiltration rate. The development of more sophisticated models will not be
described here. Instead, we will consider some of the other simple models of
infiltration which are more easily parametrised.

5.3.4 Horton’s equation and Philip’s equation

The Richards’ equation has the advantage of being physically motivated, but often
in practice, due to the difficulty in parametrising it, it is overlooked in favour of
simpler models. Empirical models have been developed based on experimental
data to describe the infiltration rate \(f(t)\) into an initially dry porous medium.
The most widely used empirical model is Horton’s model (1939) of infiltration
given by
\[
f(t) = f_f + (f_0 - f_f)e^{-\alpha t},
\]
so that \(f\) decreases from its initial value \(f_0\) to its final value \(f_f\) with a decay
rate of \(\alpha\). Integrating with respect to time will yield the cumulative infiltration
\(F(t)\). It has since been shown that Horton’s equation is a particular solution of
Richards’ equation if \(K\) and \(D\) are constants.

An alternative model is the Philip model, or Philip’s equation, which is derived
by finding an analytic solution to the Richards’ equation under certain conditions.
Philip presented approximate analytic solutions to Richards’ equation for vertical
and horizontal infiltration. In the case of vertical infiltration, Philip describes the
cumulative infiltration as an infinite power series of the form
\[
F(t) = St^{1/2} + A_1t + A_2t^{3/2} + \ldots
\]

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The coefficients in the equation depend on the initial and boundary conditions as well as the soil properties. The series is commonly truncated to the first two terms, so that it is only valid for short time. The parameter $S$ is called the sorptivity, while $A_1$ is a hydraulic conductivity. Differentiating with respect to $t$ gives the infiltration rate of infiltration capacity

$$f(t) = \frac{1}{2}St^{-\frac{1}{2}} + A_1. \quad (5.3.14)$$

As $t \to \infty$ the infiltration capacity approaches the hydraulic conductivity $A_1$. Representative infiltration curves for the Horton and Philip equations are compared in figure 5.1. Note the infiltration rate is initially infinite for the Philip equation while it is constant for the Horton equation.

5.3.5 The Green-Ampt Model

The Green-Ampt Model (1911) was one of the first physically based representations of infiltration into soils. This model preceded Richards’ equation, but Richards’ equation can be reduced to the Green-Ampt model under certain assumptions. Generally, in one dimensional infiltration into a porous medium, there is a transition between a region at the residual water content, ahead of the wetting front, to a region at equilibrium water content (possibly saturated water content) behind the wetting front. In the wetting zone the water content increases from...
the residual amount to its equilibrium value. The Green-Ampt model approxi-
mates this transition, as a sharp interface between a region ahead of the wetting
front, at residual water content $\theta_r$, and a region behind the wetting front, at
saturated (equilibrium) water content $\theta_s$. If we assume an abundance of water
at the surface (ponded water conditions or constant flux above the saturated hy-
draulic conductivity), then the water content behind the wetting front will be
the saturated water content $\theta_s$, which is equal to the bed porosity assuming no
residual air. Thus, the Green-Ampt model considers a piston like infiltration of
water into an initially dry porous medium. It is assumed that the wetted region
has constant hydraulic properties $K_s$ and $\theta_s$. The model also assumes a con-
stant capillary head or matric suction at the wetting front. This suction needs
to be determined experimentally. The assumptions made are summarised in fig-
ure 5.2, which compares what might be the real dependence of $\theta$ on depth and
that assumed in the Green-Ampt model.

Depending on the assumptions made, the model can be formulated in different
ways. Here we present a derivation for vertical infiltration, loosely following
the development in ref. [60]. We consider infiltration into a semi-infinite porous
medium bounded by $z = 0$, with $z$ increasing in the downward direction. Suppose
that the pressure at the surface $z = 0$ is determined by the atmospheric pressure
and pressure of ponded liquid covering the surface. This ponded liquid may be
subject to an externally applied pressure. Thus the hydraulic head $h$ at the $z = 0$
is given by

$$h(0) = h_a + h_0,$$

(5.3.15)

where $h_a$ is the atmospheric pressure head and $h_0$ is the head corresponding to
the ponding depth and any externally applied pressure. Now suppose the moving
wetting front is at position $z = z_f$. The hydraulic head here is

$$h(z_f) = h_a - h_f - z_f,$$

(5.3.16)

where $h_f = -\psi_f$ is the capillary head (suction) at the wetting front. For a given
front position $z_f$, the Green-Ampt model has a hydraulic gradient given by

$$\frac{dh}{dz} = - \frac{h(0) - h(z_f)}{z_f} = - \frac{h_0 + h_f + z_f}{z_f},$$

(5.3.17)
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\[ K = K(\theta) \]

\[ K_s = K(\theta_s) \]

\[ \theta_s = \theta_s - \theta_r \]

\[ h(z_f) = h_a - h_f - z_f \]

\[ h(0) = h_0 + h_a \]

\[ \Delta \theta = \theta_s - \theta_r \]

\[ K = K(\theta) \]

\[ h(z) = h_a + h_0 - \left( \frac{h_0 + h_f + z_f}{z_f} \right) z. \] (5.3.18)

Using Darcy’s law and mass balance at the wetting front yields the wetting front velocity

\[ \frac{dz_f}{dt} = - \frac{K_s}{\theta_s - \theta_r} \frac{dh}{dz} = \frac{K_s}{\Delta \theta} \left( 1 + \frac{h_0 + h_f}{z_f} \right). \] (5.3.19)

Integrating this ordinary differential equation yields the Green-Ampt solution relating front position and time

\[ t = \frac{\Delta \theta}{K_s} \left( z_f - (h_0 + h_f) \ln \left( 1 + \frac{h_0 + h_f}{z_f} \right) \right). \] (5.3.20)

This solution has been widely used to analyse infiltration of water into soils and estimate the run-off generated. The equation given is in implicit form and so may be solved iteratively by a root finder. Alternatively the model can be non-dimensionalised and studied in the short and long time limits to find approximate analytic solutions. The short time behaviour will be dominated by the applied pressure and capillary pressure terms, while the long time solution will be dominated by the pressure due to gravity. It should be clear that given an explicit solution for the wetting front position as a function of time the infiltration rate \( f(t) \) and cumulative infiltration \( F(t) \) can be calculated.
5.4 Modelling of infiltration of hot water into a packed coffee bed

A complete model of the unsaturated flow of two fluids (e.g. air and water) in a double porosity medium requires mass balance equations for air and water in both the intergranular pores and the intragranular pores, along with momentum balance equations for all phases (e.g. Darcy’s law). In addition to this, full closure of the system relies on various constitutive equations defining the relationships between capillary pressure and water saturation level, hydraulic conductivity and water saturation level, interphase transfers, etc. This is without even considering the coupling of fluid flow with solute extraction (e.g. through changes in porosity or fluid density changes) or allowing for evaporation of water or solubility of air in water. Dealing with a double porosity medium, also means that the models outlined in the previous section, for a single porosity medium, need to be adapted.

The assumption of water flow only is often made, ignoring any air flow. In certain cases, where there is a hydrostatic distribution of air and resistance to flow of air is everywhere negligible, this approximation may be justified. Given the low density and viscosity of air relative to water, and provided the air cannot sustain a pressure gradient, the approximation is often made that any air in the porous medium is at atmospheric pressure, which is usually defined to be $p_a^* = 0$. Making such assumptions, along with constant fluid density, one can describe infiltration into a doubly porous medium using two Richards’ equations to model variably saturated water flow in both the intergranular and intragranular pore systems, while allowing for the transfer of between the pore systems. Such a model is presented in ref. [30] to describe the preferential movement of water in structured porous media. This simplified model still requires the hydraulic properties of the medium such as the moisture retention curve (relating capillary pressure to saturation) and hydraulic conductivity as a function of saturation to be specified.

Simulations in ref. [30] suggest that a simpler model may be employed in certain situations. The model in ref. [30] is used to simulate vertical infiltration into a dual-porosity type’ structured medium consisting of a fracture pore system with a high hydraulic conductivity and a matrix block system with a much lower hydraulic conductivity. Water infiltrates exclusively into the fracture pore system at the top of the domain and transfer to the matrix block system is proportional
to the difference between the pressure heads in the fracture system and the pores. The hydraulic properties of the fracture and matrix systems were chosen to be indicative of relatively coarse and fine textured soils respectively. Some simulations considered different matrix block sizes. Simulations with large matrix blocks showed extreme preferential flow, where water penetrated far into the fracture pore system without saturating matrix blocks, even at the surface. Transfer rate to matrix blocks was low with pressure head non-equilibrium maintained between the phases. This is unsurprising due to the relatively small surface to volume ratio of the blocks, both to facilitate transfer to the matrix blocks and resist flow in the fractures. In contrast for smaller matrix block sizes, penetration was much slower into the fracture system, while water transfer rate to matrix blocks was very high at the wetting front, while quickly it tailed off behind it. The transfer rates are sufficiently high that the system quickly approaches pressure head equilibrium between the phases. This time the much higher surface to volume ratio of the matrix blocks provides a large surface area to resist flow in the fractures while also facilitating a higher transfer rate into the smaller blocks.

These simulations suggest that, for a sufficiently small matrix block size, infiltration may be approximated by a sharp piston like front, moving into the initially dry porous bed. All pores behind the front are assumed saturated, while all pores ahead of the front remain at their initial saturation level (zero for a dry bed). If the limiting values of residual water and air saturation are known, they can replace the notions of a fully dry or fully saturated porous medium.

As discussed above, this model of infiltration of water into a porous medium was first suggested by Green and Ampt to describe infiltration of rainfall into soil.

### 5.5 Moving boundary model of hot water infiltration into a packed coffee bed

Here, a simple one-dimensional model of water infiltration into a packed coffee bed will be presented. The model is analogous to the Green-Ampt model presented above, but capillary effects have been neglected. The model is adapted to account for the double porosity nature of the bed. It is assumed that the large applied pressure dominates the infiltration. In this model, infiltration into the
5. INFILTRATION INTO A DRY COFFEE BED

bed is assumed to proceed as a sharp front, dividing the bed into two domains. Behind the front, all the pores (intergranular and intragranular) are assumed to be saturated. Ahead of the front, the bed is at its irreducible (or residual) water saturation, which we will choose to be zero. In the saturated region behind the front we assume that coffee extraction behaves as in a fully saturated coffee bed. Any changes in porosity due to extraction will be neglected with fixed values of porosity in both pore systems specified. This removes the need to specify a water transfer term between the phases. Changes in fluid density and volume due to solute concentration are similarly neglected. Bed compaction, grain swelling and carbon dioxide evacuation are also neglected in this initial model.

We model a cylindrical coffee bed of fixed height $L$ with a vertical coordinate $z^*$ varying from $z^* = 0$ at the top of the bed to $z^* = L$ at the bottom of the bed. Note this is the opposite of the coordinate system used in the previous chapters. Hot water is injected into the bed at $z^* = 0$, under an applied pressure $\Delta P$. Alternatively, the water can be injected at a constant volume flow rate $V_m$. At a given time the position of the wetting front between the water saturated and dry regions is denoted by $z^* = H^*(t^*)$. Thus the saturated region grows from an initial thickness of $H^*(t^*) = 0$ at $t^* = 0$ to a final thickness of $H^*(t^*) = L$, at $t^* = t_f^*$.

Before outlining the equations governing the infiltration process we define the total porosity of the bed as

$$\phi_T = \phi_h + \phi_l \phi_v.$$  \hspace{1cm} (5.5.1)

As mentioned earlier, we will assume that $\phi_h$ and $\phi_v$ are constants during infiltration. We assume that the equations governing infiltration are uncoupled from those governing extraction in the saturated region and so can be considered and analysed independent of the extraction equations. For the development here, we will work with pressure as a variable rather than the hydraulic head. The infiltration model consists of three equations: Darcy’s law, mass conservation of liquid in the saturated region and mass conservation of liquid at the moving front.
5.5 Moving boundary model of hot water infiltration into a packed coffee bed

5.5.1 Water infiltration equations

The equations governing water Darcy’s law and mass conservation of liquid in the saturated region are:

\[ u_h^* = -\frac{k_h}{\mu} \left( \frac{\partial p_h^*}{\partial z^*} - \rho_h g \right), \]  
\[ \frac{\partial u_h^*}{\partial z^*} = 0 \quad \text{or} \quad \frac{\partial^2 p_h^*}{\partial z^{*2}} = 0, \]  
with \[ t^* > 0, \quad 0 < z^* < H^*(t^*). \]

Note (5.5.2) is just Darcy’s law. Either of the equations in (5.5.3) express mass conservation of liquid, assuming a constant liquid density. Substituting (5.5.2) into the first equation in (5.5.3) gives the second equation, which expresses mass conservation in terms of pressure \( p_h^* \) in the intergranular pores rather than the Darcy flux \( u_h^* \). The choice of equation depends on the boundary condition used.

Mass conservation at the moving front is given by

\[ \frac{dH^*}{dt^*} = \frac{u_h^*}{\phi_T}. \]  

for \( t^* > 0 \). Boundary and initial conditions need to be supplied in order to solve the equations. Initially the saturated region has zero thickness so that

\[ H^*(0) = 0. \]

The flow boundary conditions can be expressed by specifying the pressure at bed entrance and moving front or by specifying the Darcy flux at the bed entrance and the pressure at the moving front. We will assume that either fixed pressure or fixed Darcy flux conditions can be applied. More generally these boundary conditions may be time varying functions. For a fixed applied pressure \( \Delta P \) the pressure boundary conditions are

\[ p_h^*(0, t^*) = \Delta P, \quad p_h^*(H^*(t^*), t^*) = 0. \]
The alternative specified flux condition is

\[ u_h^*(0, t^*) = \frac{V_{in}}{A} = u_{h,in} \]

\[ p_h^*(H^*(t^*), t^*) = 0, \quad (5.5.8) \]

where \( V_{in} \) is the incoming volume flow rate and \( A \) is the bed cross sectional area.

It is worth discussing at this stage the mass balance at the interface. Since the liquid has an assumed constant density, mass balance in this context is equivalent to volume balance. The volume of liquid arriving at the interface through the intragranular pores in an infinitesimal time \( \Delta t^* \), \( u_h^* A \Delta t^* \), is balanced by the volume needed to advance the wetting fronts by a distance \( \Delta H^* \) in both the intergranular pores, \( \phi_h A \Delta H^* \), and the intragranular pores, \( \phi_l \phi_v A \Delta H^* \). This balance is based on the assumption that the pressure heads in the intergranular pores and the intragranular pores equilibrate very quickly. Thus, we can see that there is a discontinuity in the pore velocity at the moving boundary, the velocity in the pores behind the front is faster than that of the moving front. This needs to be taken into consideration when considering the transport of coffee solubles during infiltration.

### 5.5.2 Coffee extraction equations

Next we specify the equations which govern the extraction of coffee in the saturated region behind the wetting front. We assume that all coffee in the grain surfaces and grain kernels is undissolved initially. We will assume a fixed porosity in both the intergranular and intragranular pore systems throughout infiltration. Thus, while extraction is likely to lead to changes in porosity, these changes will not be modelled here. This means that the constant values of porosity need to be specified. As mentioned earlier, porosity may be changing due to compaction, swelling or extraction. We can decide whether the porosity values we choose are reflective of the porosity values at the start or end of infiltration, or an averaged value. We have four equations to track transport of coffee during infiltration:

Coffee conservation in the solution in the intergranular and intragranular pores and conservation of coffee on the grain surfaces and in the grain kernels. Thus
we have:

\[
\begin{align*}
\frac{\partial c_h^*}{\partial t^*} &= -\frac{u_h^*}{\phi_h} \frac{\partial c_h^*}{\partial z^*} + \frac{D_h}{\phi_h} \frac{\partial^2 c_h^*}{\partial z^{*2}} - \frac{\alpha}{\phi_h} (c_h^* - c_v^*) + \frac{\beta}{\phi_h} (c_{sat} - c_h^*) \psi_s^*, \\
\frac{\partial c_v^*}{\partial t^*} &= \frac{\alpha}{(1 - \phi_h) \phi_v} (c_h^* - c_v^*) + \frac{\gamma}{\phi_v} (c_{sat} - c_v^*), \\
\frac{\partial \psi_s^*}{\partial t^*} &= -\frac{\beta r_s}{(1 - \phi_h) c_s} (c_{sat} - c_h^*) \psi_s^*, \\
\frac{\partial \psi_v^*}{\partial t^*} &= -\frac{\gamma r_v}{c_s} (c_{sat} - c_v^*) \psi_v^*,
\end{align*}
\]  

(5.5.9) (5.5.10) (5.5.11) (5.5.12)

with

\[ t^* > 0, \quad 0 < z^* < H^*(t^*). \]  

(5.5.13)

The initial conditions for the fractions of the original coffee left on the surface are

\[ \psi_s^*(z^*, 0) = 1 \quad \psi_v^*(z^*, 0) = 1 \]  

(5.5.14)

for \( 0 < z^* < L^* \). The boundary condition for coffee concentration at the bed entrance is

\[ c_h^*(0, t^*) = 0, \]  

(5.5.15)

which corresponds to zero coffee concentration in the incoming water. Note this also serves as an initial condition when \( t^* = 0 \). The boundary conditions at the wetting front require a little more consideration. As discussed above, it is assumed that liquid at the moving front is instantaneously sucked into the dry grains saturating them. It is natural to assume that this fluid carries dissolved coffee with it into the intragranular pores at the same concentration it is in the intergranular pores. It is not known how well this represents the real physical process. It is suggested in ref. [68] that dry coffee grains may initially selectively absorb water from the coffee solution, before coffee solution is absorbed and free to move in and out of grains. Sample calculations assume that spent coffee grounds contain twice their mass of water and that one third of this is bound (selectively absorbed) water. This phenomenon would result in further concentrating the coffee solution in the intergranular pores. It may also lead to a delayed wetting of the grains. Here, we make the assumption that the water sucked into the grains carries all its soluble coffee with it and neglect the effects of selective absorption.
5. INFILTRATION INTO A DRY COFFEE BED

The mass balance of coffee at the wetting front \( z^* = H^*(t^*) \) gives

\[
\left( \phi_h c_{h}^* + (1 - \phi_h) c_{v}^* \right) \bigg|_{z^* = H^*(t^*)} = \frac{\mathrm{d} H^*}{\mathrm{d} t^*} \left( u_h^* c_{h}^* - \phi_h \bar{D}_h \frac{\partial c_{h}^*}{\partial z^*} \right) \bigg|_{z^* = H^*(t^*)}.
\]  

(5.5.16)

This can be further simplified by assuming that there is no diffusion at the boundary, so that the spatial derivative is zero:

\[
\left. \frac{\partial c_{h}^*}{\partial z^*} \right|_{z^* = H^*(t^*)} = 0.
\]  

(5.5.17)

Then using equations (5.5.5) and (5.5.1) it can be shown that

\[
c_{v}^*(H^*(t^*), t^*) = c_{h}^*(H^*(t^*), t^*).
\]  

(5.5.18)

It follows that at \( t^* = 0 \) and \( H^*(0) = 0 \), we get

\[
c_{v}^*(0, 0) = c_{h}^*(0, 0) = 0,
\]  

(5.5.19)

which gives an initial condition for \( c_{v}^* \).

5.5.3 Coordinate transform to immobilise wetting front

It is more convenient to work in a fixed spatial domain, particularly if we wish to solve our system numerically. For this reason we make the following change of variables to transform the problem onto a fixed domain:

\[
\xi = \frac{z^*}{H^*(t^*)}.
\]  

(5.5.20)

This leads to the following changes in the differential operators in the system:

\[
\frac{\partial}{\partial t^{*}} = -\frac{\xi}{H^*(t^*)} \frac{\mathrm{d} H^*}{\mathrm{d} t^*} \frac{\partial}{\partial \xi} + \frac{\partial}{\partial t^{*}},
\]  

(5.5.21)

\[
\frac{\partial}{\partial z^{*}} = \frac{1}{H^*(t^*)} \frac{\partial}{\partial \xi},
\]  

(5.5.22)

\[
\frac{\partial^2}{\partial z^{*2}} = \frac{1}{H^*(t^*)^2} \frac{\partial^2}{\partial \xi^2}.
\]  

(5.5.23)
5.5 Moving boundary model of hot water infiltration into a packed coffee bed

5.5.3.1 Water infiltration equations

We can rewrite the equations governing the water infiltration using the coordinate transform. First of all Darcy’s law and water mass conservation are given by:

\[ u_h^* = -\frac{k_h}{\mu} \left( \frac{1}{H^*(t^*)} \frac{\partial p_h^*}{\partial \xi} - \rho_h g \right), \]
\[ (5.5.24) \]
\[ \frac{\partial u_h^*}{\partial \xi} = 0 \quad \text{or} \quad \frac{\partial^2 p_h^*}{\partial \xi^2} = 0, \]
\[ (5.5.25) \]

with

\[ t^* > 0, \quad 0 < \xi < 1. \]
\[ (5.5.26) \]

The equation governing mass conservation of remains unchanged:

\[ \frac{dH^*}{dt^*} = \frac{u_h^*}{\phi_T}. \]
\[ (5.5.27) \]

for \( t^* > 0 \). The initial and boundary conditions are

\[ H^*(0) = 0, \]
\[ (5.5.28) \]

and

\[ p_h^*(0, t^*) = \Delta P, \]
\[ p_h^*(1, t^*) = 0, \]
\[ (5.5.29) \]

or

\[ u_h^*(0, t^*) = u_{h,in}, \quad p_h^*(1, t^*) = 0. \]
\[ (5.5.30) \]
5. INFILTRATION INTO A DRY COFFEE BED

5.5.3.2 Coffee extraction equations

The transformed equations governing extraction and transport of coffee solubles are:

\[
\frac{\partial c^*_h}{\partial t^*} = \frac{u_h}{H^*(t^*)} \left( \frac{\xi}{\phi_h} - \frac{1}{\phi_h} \right) \frac{\partial c^*_h}{\partial \xi} + \frac{\tilde{D}_h}{\phi_h H^*(t^*)^2} \frac{\partial^2 c^*_h}{\partial \xi^2} - \frac{\alpha}{\phi_h} (c^*_h - c^*_v) + \frac{\beta}{\phi_h} (c_{sat} - c^*_h) \psi^*_s,
\]  

(5.5.31)

\[
\frac{\partial c^*_v}{\partial t^*} = \frac{\xi}{H^*(t^*)} \frac{u_h \partial c^*_v}{\phi_h \partial \xi} + \frac{\alpha}{(1 - \phi_h) \phi_v} (c^*_h - c^*_v) + \frac{\gamma}{\phi_v} (c_{sat} - c^*_v),
\]  

(5.5.32)

\[
\frac{\partial \psi^*_s}{\partial t^*} = \frac{\xi}{H^*(t^*)} \frac{u_h \partial \psi^*_s}{\phi_h \partial \xi} - \frac{\beta r_s}{(1 - \phi_h) c_s} (c_{sat} - c^*_h) \psi^*_s,
\]  

(5.5.33)

\[
\frac{\partial \psi^*_v}{\partial t^*} = \frac{\xi}{H^*(t^*)} \frac{u_h \partial \psi^*_v}{\phi_h \partial \xi} - \frac{\gamma r_v}{c_s} (c_{sat} - c^*_v) \psi^*_v,
\]  

(5.5.34)

with

\[ t^* > 0, \quad 0 < \xi < 1. \]  

(5.5.35)

The initial conditions are

\[
c^*_h(\xi, 0) = 0, \quad c^*_v(\xi, 0) = 0, \]  

(5.5.36)

\[
\psi^*_s(\xi, 0) = 1, \quad \psi^*_v(\xi, 0) = 1. \]  

(5.5.37)

for \( 0 < \xi < 1 \). The boundary conditions for the system are

\[
c^*_h(0, t^*) = 0, \quad \frac{\partial c^*_h}{\partial z^*} \bigg|_{\xi=1} = 0, \]  

(5.5.38)

\[
c^*_h(1, t^*) = c^*_v(1, t^*), \]  

(5.5.39)

\[
\psi^*_s(1, t^*) = 1, \quad \psi^*_v(1, t^*) = 1. \]  

(5.5.40)

We note that the change of coordinates, fixing the spatial domain, has introduced advection terms into the equations which account for mass added to the system as the wetting front progresses.
5.5.4 Solution to the water infiltration equations

The water infiltration equations are uncoupled from the extraction equations, so we can consider these equations separately. Solving these equations, we can find the position of the wetting front at a given time and the time taken to saturate the bed. We can also solve for the pressure and Darcy flux in the saturated bed. This information can then be used in the extraction equations. We will consider two cases:

1. Boundary condition of fixed Darcy flux at the bed entrance.

2. Boundary condition of fixed applied pressure at the bed entrance.

While the fixed flux boundary condition produces a much simpler solution, the applied pressure boundary condition is more physically accurate.

5.5.4.1 Fixed Darcy flux boundary condition.

The solution for the Darcy flux in the bed is trivial. From equation (5.5.25) we find that

$$u_h^* (\xi, t^*) = f_1 (t).$$  \hspace{1cm} (5.5.41)

Then boundary condition $u_h^* (0, t^*) = u_{h, \text{in}}$ we find that

$$u_h^* (\xi, t^*) = u_{h, \text{in}}. \hspace{1cm} (5.5.42)$$

Thus we have a constant water velocity throughout the saturated region of the bed which is simply equal to the incoming velocity. Substituting this into the equation governing $H^* (t^*)$ gives us a wetting front which advances linearly in $t^*$:

$$H^* (t^*) = \frac{u_{h, \text{in}}}{\phi_T} t^*. \hspace{1cm} (5.5.43)$$

Next substituting into (5.5.24) for $u_h^*$ and $H^* (t^*)$ we find

$$\frac{\partial p_h^*}{\partial \xi} = - \left( \frac{\mu u_{h, \text{in}}}{k_h} - \rho_h g \right) \frac{u_{h, \text{in}}}{\phi_T} t^*. \hspace{1cm} (5.5.44)$$

Now integrating and applying the pressure boundary at $\xi = 1$ we find

$$p_h^* (\xi, t^*) = \frac{u_{h, \text{in}}}{\phi_T} \left( \frac{\mu u_{h, \text{in}}}{k_h} - \rho_h g \right) (1 - \xi) t^*. \hspace{1cm} (5.5.45)$$
5. INFILTRATION INTO A DRY COFFEE BED

These solutions are valid until the wetting front reaches the bottom of the bed. The time this happens is given by

\[ t_f^* = \frac{\phi T L}{u_{h, in}}. \]  \hspace{2cm} (5.5.46)

Note, the pressure is a linear function of \( \xi \), increasing from a zero value at the wetting front to a maximum value at the bed entrance. This maximum value increases linearly in time to account for the increasing bed resistance, thus maintaining a constant pore velocity. The pressure distribution at \( t^* = t_f^* \) corresponds to that during the steady state stage of extraction. Thus, in the case of a fixed Darcy flux at the bed entrance, it is straightforward to find the location of the wetting front and bed saturation time.

### 5.5.4.2 Fixed pressure boundary condition

The solution in the case of a fixed applied pressure at the bed entrance is more complex. Integrating (5.5.25) twice and applying the pressure boundary conditions gives

\[ p_h^*(\xi, t^*) = \Delta P (1 - \xi). \]  \hspace{2cm} (5.5.47)

Substituting this into Darcy’s law gives

\[ u_h^*(\xi, t) = \frac{k_h}{\mu} \left( \frac{\Delta P}{H^*(t^*) + \rho_h g} \right). \]  \hspace{2cm} (5.5.48)

Now substituting this into (5.5.27) gives

\[ \frac{dH^*}{dt^*} = \frac{k_h}{\mu \phi_T} \left( \frac{\Delta P}{H^*(t^*) + \rho_h g} \right), \]  \hspace{2cm} (5.5.49)

with \( H^*(0) = 0 \). Once a solution for \( H^*(t) \) is obtained the solutions for \( u_h^*(\xi, t^*) \) follows immediately.

First we will nondimensionalise the wetting front equation to identify the relative importance of the terms for the parameter values we are interested in. Rewriting (5.5.49) gives:

\[ H^* \frac{dH^*}{dt^*} = \frac{k_h \Delta P}{\mu \phi_T} \left( 1 + \frac{\rho_h g}{\Delta P} H^* \right), \]  \hspace{2cm} (5.5.50)
with

\[ H^*(0) = 0. \] (5.5.51)

The equations for Darcy flux and pressure are

\[ u^*_h(\xi, t^*) = \frac{k_h}{\mu} \left( \frac{\Delta P}{H^*(t^*)} + \rho_h g \right), \] (5.5.52)

\[ p^*_h(\xi, t^*) = \Delta P (1 - \xi). \] (5.5.53)

We set

\[ H^*(t^*) = LH(t), \quad t^* = \frac{L^2 \mu \phi_T}{\Delta P k_h} t, \] (5.5.54)

\[ u^*_h(\xi, t^*) = \frac{k_h \Delta P}{\mu L} u_h(\xi, t), \quad p^*_h(\xi, t^*) = \Delta P p_h(\xi, t). \] (5.5.55)

The choice of timescale reflects the dominance of the applied pressure over the hydrostatic pressure in determining the front movement. Thus the non-dimensionalised equations are

\[ H \frac{dH}{dt} = (1 + \epsilon H), \] (5.5.56)

with

\[ H(0) = 0, \] (5.5.57)

and

\[ u_h(\xi, t) = \frac{1}{H(t)} + \epsilon, \] (5.5.58)

\[ p_h(\xi, t) = 1 - \xi. \] (5.5.59)

The wetting front equation can be solved to find the implicit equation

\[ H - \frac{1}{\epsilon} \ln (1 + \epsilon H) = ct, \] (5.5.60)

where

\[ \epsilon = \frac{\rho_h g L}{\Delta P} \ll 1. \] (5.5.61)

Note for parameters reflective of the packed coffee beds considered here, \( \rho_h \sim 10^3 \), \( g \sim 10 \), \( L \sim 0.05 \) and \( \Delta P \sim 10^5 \) gives \( \epsilon \sim 0.005 \). Thus, the applied pressure
dominates infiltration as long as the bed thickness obeys

\[ L \ll \frac{\Delta P}{\rho g}. \tag{5.5.62} \]

The hydrostatic pressure only becomes significant at lower applied pressures or for much deeper beds. The dimensionless saturation time in this case is given by

\[ t_f = \frac{1}{\epsilon} - \frac{1}{\epsilon^2} \ln (1 + \epsilon). \tag{5.5.63} \]

5.5.4.3 Fixed applied pressure: Wetting front solution in terms of the Lambert W-function

The front position \( H(t) \) can be written explicitly using the Lambert W-function (Also known as the ProductLog function). The W-function is defined as the function \( W(z) \), which satisfies

\[ W(z)e^{W(z)} = z, \tag{5.5.64} \]

for any complex number \( z \). More detail on the Lambert W-function can be found in ref. [17].

For \( z = x \in \mathbb{R} \), the W-function is only defined for \( x \geq -e^{-1} \) and double valued for \( -e^{-1} < x < 0 \). For \( W \geq -1 \) we can define a single valued function \( W_0(x) \) with \( W_0(0) = 0 \) and \( W_0(-e^{-1}) = -1 \). This is the upper branch of the function.

The lower branch of the function for \( W \leq -1 \) is denoted by \( W_{-1}(x) \). It decreases from \( W_{-1}(-e^{-1}) = -1 \) to \( W_{-1}(0^-) = -\infty \). The two branches of the Lambert W-function for real values \( x \geq -e^{-1} \) are shown in figure 5.3. Here we will use the lower branch of the function to describe the position of the wetting front.

First, we rewrite equation (5.5.60) in the following form:

\[ -(1 + \epsilon H) + \ln (1 + \epsilon H) = -(1 + \epsilon^2 t). \tag{5.5.65} \]

Next, we apply the exponential function to both sides and simplify:

\[ -(1 + \epsilon H)e^{-(1+\epsilon H)} = -e^{-(1+\epsilon^2 t)}. \tag{5.5.66} \]
5.5 Moving boundary model of hot water infiltration into a packed coffee bed

Now setting

\[ W(t) = -(1 + \epsilon H), \quad (5.5.67) \]
\[ x(t) = -e^{-(1+\epsilon^2 t)}, \quad (5.5.68) \]

we have reduced the problem to solving the defining equation of the Lambert W-function for \( W \leq -1 \) and \( -e^{-1} \leq x < 0 \). This solution is given by the lower branch function \( W_{-1}(x) \). Thus the solution is

\[ H(t) = -\frac{1}{\epsilon} \left( 1 + W_{-1}( -e^{-(1+\epsilon^2 t)} ) \right). \quad (5.5.69) \]

The solution in dimensional variables is

\[ H^*(t^*) = -\frac{\Delta P}{\rho_h g} \left( 1 + W_{-1} \left( -e^{\left(1+\frac{\epsilon^2 g^2}{\Delta P \rho_h h}\right) t^*} \right) \right). \quad (5.5.70) \]

5.5.4.4 Fixed applied pressure: Wetting front solution in terms of an asymptotic expansion

An alternative to using the Lambert W-function, is to make use of the small parameter \( \epsilon \), to construct an asymptotic solution to (5.5.56). We use the following
regular expansion for the wetting front position:

\[ H(t) \sim H_0(t) + \epsilon H_1(t) + \epsilon^2 H_2(t) + \epsilon^3 H_3(t). \]  

(5.5.71)

Making the substitution and solving the equations at each order gives the following asymptotic solution:

\[ H(t) = \sqrt{2t} + \epsilon \left( \frac{2t}{3} \right) + \epsilon^2 \left( \frac{t^3}{9\sqrt{2}} \right) + \epsilon^3 \left( -\frac{2t^2}{135} \right) + O(\epsilon^4). \]  

(5.5.72)

Figure 5.4 compares the Lambert W-function to asymptotic solutions to different orders for \( \epsilon \sim 0.005 \). It is clear that for the values \( \epsilon \sim 0.005 \) typical for the packed beds in the cylindrical flow cell experiment under consideration even the leading order term gives a good agreement to the exact solution over the time domain of interest. This is due to the dominance of the driving pressure over the gravity driven term in the shallow bed. Figure 5.5 makes the same comparison for a value of \( \epsilon = 0.5 \). In this case the gravity driven term becomes more influential as the wetting front nears the bed exit. Since this term is neglected at leading order we can see the leading order term underestimates the front position.
5.6 Numerical simulation of extraction during infiltration into coffee bed

Substituting for $H(t)$ in equation (5.5.58) gives us the Darcy flux. We note that the Darcy flux has a singularity at $t = 0$ since $H(0) = 0$. Thus $u_h$ rapidly decreases from an infinite value at $t = 0$, before reaching its steady state value at $t = t_f$, when $H(t) = 1$:

$$u_h(\xi, t_f) = \frac{1}{L} + \epsilon. \quad (5.5.73)$$

It is worth noting that for an infinitely deep bed, the driving pressure term tends to zero for large $H(t)$ and the gravity driven term drives the flow. For a value $\epsilon = 0.005$ the Darcy flux is plotted in figure 5.6.

In reality the initial flux of water into the bed must be bounded. For the experiments outlined earlier this bound is specified by the maximum flow rate of the pump for a given pressure.

5.6 Numerical simulation of extraction during infiltration into coffee bed

In the previous section, we analysed the equations governing the position of the wetting front and the fluid velocity during infiltration. The solutions to these equations, allow us to specify the domain on which extraction is occurring during
the wetting stage of the brewing process. The next step is to consider the equations governing coffee extraction and transport in this domain. The equations outlined earlier consist of four coupled non-linear partial differential equations. The solutions obtained for \( H^* (t^*) \), \( u^*_h (\xi, t^*) \) and \( p^*_h (\xi, t^*) \), can be substituted into the equations. In this section, numerical solutions to the dimensional equations, with parameters corresponding to those used for a fine grind (JK standard drip filter coffee) and a coarse grind (Cimbali # 20) in the steady state stage, are presented. These solutions will be compared under the two boundary conditions discussed earlier. Some comparison will also be made with the initial conditions used for the steady state stage for these grinds. Full non-dimensionalisation and in-depth analysis of the equations will not be presented here and results shown should be viewed in the context of the assumptions made. The model requires more development before the results it produces are seen to be any more reliable than the estimates of the coffee concentration profiles following infiltration.

For the numerical simulations presented here, we will assume that transport of coffee solubles by diffusion in the saturated intergranular pores is negligible in comparison with transport via advection. The initial condition of the wetting front position \( H^* (0) = 0 \), leads to an undefined initial pressure gradient and initial Darcy flux. To overcome this issue, we start the simulations at small time \( t^*_{init} > 0 \), but with \( t^*_{init} \ll t^*_f \). As we have already solved the equation for the
5.6 Numerical simulation of extraction during infiltration into coffee bed

wetting front position, we can calculate the new ‘initial’ position $H^*(t_{\text{init}}^*)$. Thus the system is initialised with a narrow water saturated region. We assume that no coffee has yet extracted into the water in this region. For a sufficiently small value of $t_{\text{init}}^*$, the error introduced by this approximation should be negligible. Thus we will solve the extraction equations for $t_{\text{init}}^* < t^* < t_f^*$. The main outputs of interest from the simulations will be the coffee concentration profiles in the two pore systems and the fractions of soluble coffee left on the grain surfaces and in the grain kernels at $t^* = t_f^*$. These results can be compared with the assumed initial conditions for the steady state stage extraction. Thus the equations for simulation are

\[
\frac{\partial c_h^*}{\partial t^*} = \frac{u_h^*}{H^*(t^*)} \left( \frac{\xi}{\phi_h} - \frac{1}{\phi_h} \right) \frac{\partial c_h^*}{\partial \xi} - \frac{\alpha}{\phi_h} (c_h^* - c_v^*) + \frac{\beta}{\phi_h} (c_{\text{sat}} - c_h^*) \psi_s^*, \tag{5.6.1}
\]

\[
\frac{\partial c_v^*}{\partial t^*} = \frac{\xi}{H^*(t^*)} \frac{\partial c_v^*}{\partial \xi} - \frac{\alpha}{\phi_v} (1 - \phi_h) (c_h^* - c_v^*) + \frac{\gamma}{\phi_v} (c_{\text{sat}} - c_v^*) \psi_s^*, \tag{5.6.2}
\]

\[
\frac{\partial \psi_s^*}{\partial t^*} = \frac{\xi}{H^*(t^*)} \frac{\partial \psi_s^*}{\partial \xi} - \frac{\beta r_s}{(1 - \phi_h)c_s} (c_{\text{sat}} - c_h^*) \psi_s^*, \tag{5.6.3}
\]

\[
\frac{\partial \psi_v^*}{\partial t^*} = \frac{\xi}{H^*(t^*)} \frac{\partial \psi_v^*}{\partial \xi} - \frac{\gamma r_v}{c_s} \psi_s^*, \tag{5.6.4}
\]

with

\[ t^* > t_{\text{init}}^*, \quad 0 < \xi < 1. \tag{5.6.5}\]

The initial conditions are

\[
c_h^*(\xi, t_{\text{init}}^*) = 0, \quad c_v^*(\xi, t_{\text{init}}^*) = 0, \tag{5.6.6}
\]

\[
\psi_s^*(\xi, t_{\text{init}}^*) = 1, \quad \psi_v^*(\xi, t_{\text{init}}^*) = 1, \tag{5.6.7}
\]

for $0 < \xi < 1$. The boundary conditions for the system are

\[
c_h^*(0, t^*) = 0, \quad c_h^*(1, t^*) = c_h^*(1, t^*), \tag{5.6.8}
\]

\[
\psi_s^*(1, t^*) = 1, \quad \psi_v^*(1, t^*) = 1. \tag{5.6.9}
\]

The solutions for $H^*(t^*)$ and $u_h^*(\xi, t^*)$ are known and can be substituted into the equations (or alternatively solved explicitly in the numerical scheme). Here the
system is solved by partitioning the $\xi$ domain into discrete points and writing derivatives in $\xi$ using finite differences. This reduces the problem to a system with four ordinary differential equations at each point in the discretisation of $\xi$. The values at the boundary points are assigned according to the boundary conditions. We can then solve this system using a standard solver for ODEs.

### 5.6.1 Wetting front position and velocity

The dynamics of the wetting front position and velocity differs depending on the boundary condition applied and of course the bed properties. The applied pressure in the experiments was chosen to achieve a specific volume flow rate at steady state, in this case 250 mL min$^{-1}$, to achieve a brewing time of approximately four minutes for one litre of water. Thus the applied pressure was 2.3 bar for the fine grind and 0.65 bar for the coarse grind are used. The volume flow rate in the bed decreases from its maximum value as the bed resistance increases until it reaches its steady value when the bed is saturated. The pump’s maximum flow rate is not accounted for in our model so the initial flow rate will be higher than in reality until the bed resistance reduces the flow below the pump’s maximum flow rate.

The fixed flux condition assumes that the specified flow rate of 250 mL min$^{-1}$ is achieved throughout the infiltration time, the applied pressure adjusting itself to maintain a fixed flow rate as the bed resistance increases. If the steady state flow rate is used during infiltration, infiltration under the fixed flux boundary condition will take longer than the fixed applied pressure boundary condition, since the flow rate is always lower except at the point of saturation.

The boundary conditions and selected parameters used for the simulations that will be presented here are shown in table 5.1. Also shown are some of the key parameters. Note the value used for the intragranular porosity is that of the grain porosity when all soluble coffee has been dissolved. This choice of parameter may lead to a longer infiltration time than expected. As expected the saturation time is much shorter for the applied pressure B.C. The saturation time is slightly longer for the bed of course grounds under both boundary conditions. This can be attributed to the greater bed depth due to less compaction.

The wetting front positions for the four different simulations are shown in figure 5.7. When the applied pressure is fixed, the front advance is approximately proportional to $\sqrt{t}$. When the volume flow rate is fixed, the front moves into the
5.6 Numerical simulation of extraction during infiltration into coffee bed

<table>
<thead>
<tr>
<th></th>
<th>Fine Grind</th>
<th>Coarse Grind</th>
</tr>
</thead>
<tbody>
<tr>
<td>B.C.</td>
<td>Pressure</td>
<td>Flux</td>
</tr>
<tr>
<td>Upper B.C.</td>
<td>2.3 bar</td>
<td>250 mL min⁻¹</td>
</tr>
<tr>
<td>Bed Depth</td>
<td>0.0405 m</td>
<td>0.0405 m</td>
</tr>
<tr>
<td>φₜₜ</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>φₜ∞</td>
<td>0.7034</td>
<td>0.7034</td>
</tr>
<tr>
<td>φₜ</td>
<td>0.7627</td>
<td>0.7627</td>
</tr>
<tr>
<td>tₚ</td>
<td>10.2216 s</td>
<td>20.2689 s</td>
</tr>
</tbody>
</table>

Table 5.1: Boundary conditions and selected parameters for infiltration simulations

bed at a constant rate and so its advance is proportional to \( t^* \). In either case, the pressure is a linear function of the transformed coordinate \( \xi \), varying from the applied pressure at the bed entrance to zero at the wetting front. The applied pressure in the fixed flux case, increases linearly in \( t^* \). These functions have been shown in (5.5.53) and (5.5.45) and, given their simple form, are not plotted here.

![Figure 5.7: Comparison of wetting front position for infiltration under fixed applied pressure and fixed applied flux into packed coffee beds of (a) fine grinds and (b) coarse grinds.](image)

The velocity of the wetting front can be got from the Darcy flux \( u^*_h \), by dividing by the total porosity \( \phi_T \). For a fixed applied pressure, the Darcy flux is a decreasing function of \( t^* \), while for a fixed applied flux, it is constant and equal to the applied flux. The Darcy flux during infiltration is plotted for each of the four simulations in figure 5.8.
5. INFILTRATION INTO A DRY COFFEE BED

5.6.2 Coffee extraction during infiltration

5.6.2.1 Coffee solubles transport during infiltration

As the wetting front propagates into the coffee bed, coffee solubles in the saturated grains behind the front begin to extract into the water, in both the intergranular and intragranular pores. Solubles enter the saturated intragranular pores as the solids dissolve from the cell walls into the cell lumens. Solubles can enter the intergranular pores by direct dissolution from broken cells on the grain surfaces or from the intragranular pores via diffusion through the grains cellular matrix. Once the solubles enter the intergranular pores, they can be transported down through the bed via advection. At the wetting front, coffee solution is sucked into the dry coffee cells, carrying with it coffee solubles.

The rates at which these processes occur has been assumed to correspond to the fitted coefficients in the steady state stage. Of course this is not necessarily correct. Further, these fitted coefficients may be dependent on the choice of initial conditions made for the steady state stage in the first place. Clearly it would be preferable to fit both models at the same time, achieving the best fit to both models. Here, we will just compare the output of the infiltration model with the initial conditions assumed for the steady state stage in previous chapters. The next step would be attempting to fit the new extended model (now including
infiltration) to available data. In order for the model to be useful, its ability to capture the dynamics of infiltration should be verified by experiment. Since there is very little data currently available to us on water flow during infiltration and none on coffee extraction, this step will not be attempted here.

5.6.2.2 Coffee concentrations following infiltration

Once infiltration is complete, we can plot the solutions for coffee concentrations in the intergranular and intragranular pores and compare them for the different simulations. Figure 5.9a compares the coffee concentrations in the intergranular pores across the four simulations. It can be seen that the concentration in the intergranular pores is much higher in the fine grind simulations. This can be attributed to the greater surface area for extraction, coupled with a greater proportion of soluble coffee adjacent to the coffee surfaces in the fine coffee grind.

Some differences are also observed for the different boundary conditions. The coffee concentration is slightly higher in the case of the fixed applied pressure boundary condition for both coffee grinds. The reason for this is the longer infiltration time $t_f^*$ in the fixed flux case. This may seem a little counter-intuitive. One would expect a longer extraction time to lead to increased extraction and a higher concentration. More extraction does occur from the grain surfaces but the longer extraction time means coffee is sucked into the grains at a higher concentration, at lower values of $H^*(t^*)$.

Figure 5.9b compares the concentration in the intragranular pores for the four simulations. Again higher concentrations are observed in the case of the fine grind simulations, although the concentrations are actually lower near the bed entrance. There are a number of reasons for this. The reason for the overall higher levels of coffee in the intragranular pores in the case of the fine grind, is the suction of coffee solution, at a higher concentration into the grains. This leads to a higher concentration in the grains, despite the fact that the levels of soluble coffee in the grain kernels is actually less for the fine grind. The reason for the lower concentration at the bed entrance is because surface coffee did not have time to extract before the water was sucked into the grains near the bed entrance. Thus the lower levels here are reflective of the lower levels of soluble coffee in the grain kernels.

We also note the differences between the two boundary conditions simulated. Concentrations are higher for the fixed flux boundary condition. As outlined
5. INFILTRATION INTO A DRY COFFEE BED

Figure 5.9: Comparison of coffee concentrations following infiltration. Coffee concentrations in (a) the intergranular pores and (b) the intragranular pores are plotted for each of the four simulations. In the case of the fixed applied pressure boundary condition, the concentrations in both pores systems are compared for (c) the fine grind and (d) the coarse grind.

above, this is due to the increased infiltration time, allowing for more surface coffee to extract, before being sucked into the intragranular pores.

Figures 5.9c and 5.9d compare the intergranular and intragranular concentrations in the case of the fixed applied pressure boundary condition for the fine and coarse grinds. The concentration in the intergranular pores effectively provides the initial condition for concentration in the intragranular pores, so, it is not surprising to see the concentration is higher in the intragranular pores. Dissolution of coffee from the cell walls inside the grains, drives the higher concentration in these pores. This concentration reaches close to saturation level in the fine grind, but not in the course grind.
5.6.2.3 Comparison to estimated initial conditions for steady state stage

The simulated concentration profiles following infiltration can now be compared with the initial conditions assumed in previous chapters. This comparison is made in figure 5.10. Figure 5.10a shows the comparison for the concentration $c_h^*$ in the case of the fine grind. It had been assumed that the concentration in the intergranular pores was approximately at coffee saturation level following infiltration. Noting that coffee concentration exiting the bed during experiments was near the assumed saturation level, this was based on the assumption of rapid surface extraction, coupled with large flow resistance, meaning coffee would extract much faster than it could be advected away, during infiltration. However, the suction of coffee solution into the grains, was not taken into account. This leads to a much lower assumed initial concentration in the grains compared to simulation results, as illustrated in figure 5.10b. Also no attempt was made to prescribe the dependence of concentration on depth in the intragranular pores.

In the case of the coarse grind, figure 5.10c shows that the assumed initial condition agrees quite well with the simulated result. In this case, the assumption was made that the smaller surface to volume ratio of the grain distribution would lead to a dominance of advection over surface extraction, so that coffee could be carried away in the flow as fast as it was dissolving. Thus the linear build up of coffee solubles with bed depth is the result of advection. The linear profile was fixed using the observed initial exiting concentrations from experiment. Again transfer of coffee solubles into the grains was not accounted for. Figure 5.10d compares the estimated and simulated profiles for $c_v^*$. The shape of the $c_v^*$ curves from simulations are due to the suction of coffee solution into the grains and again this was not accounted for in the initial estimates.

5.6.2.4 Remaining soluble coffee following infiltration

The other quantities of interest are the fractions of soluble coffee remaining in the grain surfaces and in the grain kernels following infiltration. In figure 5.11a the fraction of soluble coffee remaining in the grain surfaces following infiltration is plotted. It can be clearly seen that the surface coffee in the fine grind is more depleted, in line with its greater surface area for extraction. Also, as $c_h^*$ increases, as the wetting front approaches the bed exit, surface coffee is largely undissolved
here, due to a smaller driving concentration gradient as well as a shorter contact time. Surface coffee just at the bed exit, which has only just been contacted with water, is completely undissolved. Despite a longer exposure a higher level of surface coffee remains in the coarse grind due to its much smaller grain surface area.

Figure 5.10 shows the corresponding plot for the fraction of soluble coffee remaining in the grain kernels. The coffee solubles in the coarse grounds are more depleted. This is reflective of the fact that these solubles have a longer contact time. Unlike the grain surfaces, there is no reason for there to be a difference in the surface area (per unit volume) available for extraction in the grain kernels of

\[ c_{\text{sol},i}(\xi, t_f^*) \] (kg/m³)

\[ c_{\text{sol},i}(\xi, t_f^*) \] (kg/m³)

\[ c_{\text{sol},i}(\xi, t_f^*) \] (kg/m³)

\[ c_{\text{sol},i}(\xi, t_f^*) \] (kg/m³)
5.6 Numerical simulation of extraction during infiltration into coffee bed

The results for the fraction of coffee solubles remaining in the two regions in the
grains are compared with the initial conditions assumed for the steady state stage
in figure 5.12. The simulations show that more solubles were extracted from the
grain surfaces during infiltration than was assumed. This is expected, as the
earlier estimates did not allow for the suction of coffee soluble into the grains.
Also the estimates did not account for spatial variations in the initial conditions.

In the grain kernels, it had been assumed that all coffee solubles had been
dissolved during the infiltration stage. The simulations show that this may be
the case in the upper part of the bed, but will not be the case near the bed
exit, where contact time of water with the grains has been much shorter. The
concentration of the coffee in the water sucked into the grains is also higher nearer
the bed exit. The difference is particularly significant for the fine grind. Again,
it should be emphasised that the rate of dissolution of coffee within the grains
has not and cannot be fitted to any available data. Thus, if extraction rate is

Figure 5.11: Comparison of fractions of soluble coffee remaining following in-
filtration. Fractions of soluble coffee in (a) the grain surfaces and (b) the grain
kernels are plotted for each of the four simulations.

the fine or coarse grind. Thus larger contact time coupled with a higher driving
force (recall $c_0^*$ is lower) means the grain kernels in the coarse grains are more
depleted. It shown be noted that the value assigned to the parameter $\gamma$ here is
not fitted, since there is no data to fit from.

5.6.2.5 Comparison to estimated initial conditions for steady state
stage

The results for the fraction of coffee solubles remaining in the two regions in the
grains are compared with the initial conditions assumed for the steady state stage
in figure 5.12. The simulations show that more solubles were extracted from the
grain surfaces during infiltration than was assumed. This is expected, as the
earlier estimates did not allow for the suction of coffee soluble into the grains.
Also the estimates did not account for spatial variations in the initial conditions.

In the grain kernels, it had been assumed that all coffee solubles had been
dissolved during the infiltration stage. The simulations show that this may be
the case in the upper part of the bed, but will not be the case near the bed
exit, where contact time of water with the grains has been much shorter. The
concentration of the coffee in the water sucked into the grains is also higher nearer
the bed exit. The difference is particularly significant for the fine grind. Again,
it should be emphasised that the rate of dissolution of coffee within the grains
has not and cannot be fitted to any available data. Thus, if extraction rate is

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5. INFILTRATION INTO A DRY COFFEE BED

significantly slower (or faster) the resulting profile will be changed accordingly.

![Graphs showing infiltration into a dry coffee bed](image)

**Figure 5.12:** Comparison of fractions of soluble coffee remaining following infiltration with estimated initial conditions for the steady state stage. Simulated fractions of soluble coffee remaining for the fine grind in (a) the grain surfaces and (b) the grain kernels are plotted alongside earlier estimates. Simulated fractions of soluble coffee remaining for the coarse grind in (c) the grain surfaces and (d) the grain kernels are plotted alongside earlier estimates.

### 5.7 Discussion and conclusions

The purpose of this chapter, was to give some consideration to the infiltration or filling stage of coffee brewing in a packed bed. Modelling of this part of the brewing process had been neglected in previous chapters, requiring the initial forms of the different variables following infiltration to be prescribed. The only aid in deciding the form of these variables was the concentration data collected...
from the exiting coffee solution after infiltration is complete. This means even if
the guessed forms are correct, by luck or otherwise, it is difficult to extrapolate
them to beds with different parameters. The difficulty on improving on this
process lies in the absence of available data on which to hypothesise or validate
a model. Thus the discussion and development here should be seen as an initial
exploration of the problem rather than the creation of a reliable model.

To this end, we have made a number of assumptions about the infiltration
process, chief among them being that the infiltration can be modelled as a sharp
piston like front, moving into the dry coffee bed. The front divides the bed into a
fully saturated domain and a fully unsaturated domain. This assumption removes
the need to specify unknown constitutive relationships between variables, like
defining capillary pressure and hydraulic conductivity as a function saturation.
If the transition between the fully saturated and dry coffee bed occurs over a short
distance this assumption may give reasonable results. The movement of the front
is controlled by mass (volume) balance at the wetting front (i.e. the wetting front
must fill all available void space as it proceeds), and of course infiltration rate
into the porous medium. Once the saturated domain is established, we simply
apply the already established extraction equations in this domain, while taking
care to ensure conservation of coffee at the wetting front.

The water infiltration equations governing the wetting front position, water
velocity and pressure have been considered and solved under two different bound-
ary conditions governing the injection of fluid at the upper boundary. In the case
of a fixed applied fluid flux, the solution is trivial. For a fixed applied pressure,
the problem is non-dimensionalised and solved exactly in terms of the Lambert-W
function. An asymptotic solution is also presented based on the small parameter
describing the ratio of the maximum hydrostatic pressure to the applied pressure
at the bed entrance.
Part II

Mathematical modelling of a contact lens hydration process
6.1 Introduction

The work in this part of the thesis was carried out as part of a one year research programme funded by Johnson & Johnson. The work was undertaken in consultation with design and process engineers at Johnson & Johnson company Vistakon. Based on the requirements of the industry partner, significant effort was made to connect the models developed with available experimental data. Much time was also spent adapting models to numerous design changes in the considered process. Having focused on these tasks for the duration of the project, there remain possibilities for further mathematical work in simplifying and non-dimensionalising the resulting models for further analysis.

6.1.1 Contact lenses

A contact lens is a thin lens which is placed directly on the surface of the eye. Contact lenses are generally worn for vision correction, therapeutic and cosmetic purposes [22], and can be classified using various criteria. They are most commonly classified by their primary function (vision correction, cosmetic or therapeutic), material or intended period of use. Corrective lenses utilise their refractive properties to alter the direction of incident light rays in order to focus them properly.
CONTACT LENS MANUFACTURING PROCESS

Contact lenses are designed to change the appearance of the eye, although they may also serve to correct vision. Therapeutic lenses are designed to treat disorders in the eye other than the refractive properties. Contact lenses also have potential as drug delivery devices, as an alternative to eye drops [74], and as biosensors [22]. Contact lenses are classified as hard or soft according to the elasticity of their constituent materials [12]. Hard contact lenses were originally made from rigid polymer based materials such as poly(methylmethacrylate) (PMMA) [40]. More recently new materials have been developed to make rigid gas permeable (RGP) contact lenses which overcome the low oxygen permeability of PMMA lenses. Soft contact lenses are made from hydrogel or silicon-hydrogel materials. Silicon-hydrogels are now the most prevalent on the market due to their comfortable fit and higher oxygen permeability [12]. The intended period of use for contact lenses ranges from one day, for daily disposable lenses, up to a month for extended wear contact lenses.

Contact lenses are manufactured in a variety of ways. Hard contact lenses tend to be custom made and generally are manufactured using a lathe cutting process. Soft contact lenses can be manufactured using lathe-cutting, spin casting and cast-moulding [43].

In this work, we will consider a contact lens manufacturing process used by Vistakon, a division of Johnson & Johnson Vision Care. Headquartered in Jacksonville in Florida in the United States, Vistakon also has a manufacturing facility in Limerick in Ireland. The company, which produces the Acuvue brand of contact lenses, is one of the leading manufacturers of contact lenses in the world. The plant in Limerick has a number of production lines which manufacture soft contact lenses using a cast-moulding process. The production lines are almost entirely automated. The 4GT (fourth generation) production lines currently in operation can manufacture up to 180000 lenses per 12 hour shift.

6.1.2 Cast-moulding process

The cast-moulding manufacturing process used by Vistakon consists of a number of steps, performed sequentially on each production line. The first step on the production line is the manufacture of the moulds which will define the shape of the lens. The shape of the back of the lens is defined by the back curve mould. The back curve forms the male part of the mould and has a spherical shape to
fit onto the eye. The shape of the front of the lens is determined by the front curve of the mould. The front curve forms the female part of the mould and its shape determines the power of the lens. The mould sections are produced by injection moulding using a thermoplastic material. The lenses are then formed by sandwiching a liquid monomer mixture (uncured lens formulation) between the front curve (lower mould) and the back curve (upper mould). Following this, the initial reactive mixture is cured under UV light. The monomer is polymerised thus forming the lens. Typically during polymerisation of the hydrogels, the lenses tend to shrink \( [13] \). To prevent this, an inert diluent is usually included in the initial reactive mixture to fill up the spaces in the lens during polymerisation. The diluent will subsequently be replaced by water in later processing steps. This process is known as stabilised soft moulding \([38]\). After the lenses have been polymerised the back curves are removed, leaving the lenses sitting in their front curves.

### 6.1.2.1 Hydration

The next step on the production line is the hydration process. This process serves a number of purposes. Firstly the process involves the removal of any unwanted leachable material in the contact lenses. The unwanted material may include unreacted monomers, catalysts and/or partially reacted comonomers, diluents or other impurities \([3]\). The lenses are also hydrated with water during the process. Finally, the swelling the lens undergoes during the hydration process serves to detach the lens from its front curve. Thus, exiting the hydration process the lenses are hydrated, free from unwanted chemicals and detached from their front curves. The hydration process involves washing the lenses with one or more hydration fluids. The hydration fluid is absorbed by the lenses, leachable material is dissolved in the hydration fluid and leached from the lenses, driven by the concentration gradient between the fluid in the lenses and fluid in contact with the lenses. Usually the hydration fluid is maintained at a high temperature to speed up extraction. In some processes, it is sufficient just to hydrate the lenses by washing them with deionised water. Frequently, however hydration will include one or more washing steps using volatile organic solvents to remove hydrophobic chemical ingredients \([39]\). Thus hydration may consist of a number of washing stages involving leaching of certain chemicals. The last stage will involve the displacement of organic solvents in the lenses with deionised water.
The hydration process which will be studied here, involves the use of one organic solvent called propylene glycol and deionised water. This process will be outlined in detail later. A schematic of the manufacturing process up to the hydration stage is shown in figure 6.1.

Following hydration the contact lenses are quality tested and packaged for distribution. The whole process is fully automated from start to finish.

6.1.3 Cast moulding process limitations

Currently the hydration process is the rate limiting step in the production line. Thus increasing the lens throughput in the hydration process will directly increase the overall output of the production line. As the hydration process module has to fit into the existing limited footprint of the production line, simply replicating the existing process in parallel was not a viable option. For this reason, Vistakon have redesigned the lens hydration section of the production line to increase lens throughput and also to improve the efficiency of the process. The key questions to be addressed here relate to heat and chemical transport in the newly designed hydration module. Modelling of heat transport in the system is chiefly required in order to estimate the size of heating elements in the system so as to maintain the extracting fluid at required process temperatures. The location of heat energy losses needs to be identified so that heating elements can replace lost energy. Over-sizing heating elements is also undesirable due to space limitations and increased purchase and maintenance costs. Modelling of chemical transport (removal of leachables from system) in addition to heat transport is required in...
order to explore the space of process parameters, to establish the optimal process parameters to maximise the benefit of the new process. Clearly the process needs to clean lenses to the required specifications, but, within this constraint, it is desirable to minimise costs (e.g. reduce solvent required) and maximise lens throughput. In the next sections, the hydration process will be described and the key modelling questions established and presented.

6.2 5GT hydration process

6.2.1 Process description

The newly designed hydration process is part of the fifth generation (5GT) production lines to be installed in Vistakon’s manufacturing plants. In the case of interest here, the hydration process involves the removal of a chemical called 3,7-dimethyl-3-octanol (D3O) from the lenses. This chemical is used as a diluent in the initial monomer mix when manufacturing the lens. It makes up 23% of the initial lens constituents by mass. Unfortunately D3O is relatively hydrophobic and so cannot be removed with water. Also if one attempts to release the lenses in water, D3O will prevent the absorption of water and not allow sufficient swelling to cause the release of the lens [75]. Thus the hydration process in this instance is a two-stage process. The first stage involves the leaching of D3O from the lenses using an organic solvent called propylene glycol (PG). Following this, the PG is removed from the lenses by washing them with deionised water (DI). In this second stage the PG in the lenses gets replaced with the DI.

Entering the hydration module, the lenses are held in their front curve moulds in plastic trays. A lens which has been detached from its front curve is shown in figure 6.2a. Each tray has 64 hemispherical cavities, each containing a front curve with lens attached. A picture of an empty tray can be seen in figure 6.2b. Note the presence of a drainage hole at the bottom of each cavity. Figure 6.2c shows a stack of trays with front curves in place. Each of the cavities has grooves under the front curve it contains, which allows fluid to cascade down over the lenses through the tray. The trays are arranged in stacks of about 30 trays high.

In the hydration chamber the lenses are washed at a number of stations, which we will refer to as stages. Figure 6.2d shows a hydration system rig with five dosing stages. The stacks spend a fixed time (referred to as the index or cycle...
time) at each stage before moving on to the next. Each stage has its own tank and heater (to maintain the fluid at the required temperature). Each stage also has a shower, with 64 nozzles, which delivers fluid to the top of the stack of trays. When a stack of trays enters a stage, hydration fluid (PG or DI) is delivered at a fixed flow rate from the holding tank through a heater, which heats it such that it reaches process temperature before reaching the shower head. Typical flow rates may be 5 L min\(^{-1}\). This will be referred to as the circulation flow. The fluid enters the lens cavities, washes over the lenses and overflows, cascading from tray to tray down through the tower and back into the tank. The mixing between these 64 ‘columns’ in the 30 trays is negligible. The concentration of leachable chemical in the solvent in the tanks will build up over time if left unchecked, rendering the process ineffective. For this reason, fresh solvent is delivered to the tanks at a fixed flow rate, while contaminated solvent is removed at the same flow rate. This will be referred to as the refresh flow and its flow rate may differ from the circulation flow rate. A schematic of solvent flows in a typical stage is shown in figure 6.3.

The initial stages wash the lenses with pure propylene glycol (PG), to remove
the water insoluble D3O. The remaining stages wash the lenses with deionised water (DI) to remove the PG. The PG temperature needs to be maintained at a process temperature above 90°C during washing. A drop in temperature will lead to a slower extraction and may also influence the swelling and release behaviour of the lens. As PG is expensive to use and dispose of, it is undesirable to deliver fresh PG to each tank in every stage. This may also require significant energy to heat the quantity of PG required. Thus the stages are connected up, consecutively, in a series. Fresh PG is only delivered to the top of the final PG washing stage. This will be the refresh flow for the system. Here the lenses should be at their cleanest. PG exiting the stack in the final stage is collected in its tank, and overflows into the adjacent tank to refresh the second last stage. This overflow process continues from tank to tank before contaminated PG solvent is removed from the system, from the tank in the first PG stage. In each stage, the circulation flow occurs, from tank to stack and back, leaching D3O from the lenses. Thus there is a countercurrent extraction, where PG flows in one direction, getting more and more contaminated, while lenses move in the other
direction, spending a fixed time at each stage, before moving to the next. As the lenses move they get cleaner and cleaner so that the process aims to maintain the maximum concentration gradient between the D3O in the lenses and the D3O in the PG.

### 6.2.2 Factors influencing hydration

The total contact time for D3O extraction with PG, is determined largely by the time needed to allow diffusion of D3O out of the lens. Some other factors also influence the times needed. The concentration gradient should be maximised throughout extraction (this will depend on the refresh rate). Also the times over which the lenses swell and release are not known exactly. It is estimated that the time taken for PG concentration in the lenses to reach equilibrium may be 5–10 minutes. The time for release of the lens from the front curves may be as high as 20–30 minutes. The degree of swelling will likely influence the rate at which diffusion occurs from the lens. The release time may also be important, as it allows for the possibility of two-sided diffusion from the lenses, increasing the extraction rate.

Experiments, carried out by Vistakon, show that an extraction time of about 2700 s (45 minutes) for PG washing and 1800 s (30 minutes) for DI washing is required. The time spent at each stage, called the index or cycle time, is arrived at by simply dividing the total extraction time by the number of stages. Using more stages means an increased throughput, but is limited by the increased time required to move stacks between stages and by space considerations. For a hydration module with 6 PG dosing stages and 4 DI dosing stages (proposed production line specifications), the index time is 450 s. The index time is broken up into three main periods (with representative durations) as follows:

1. Dosing time (360 s).
2. Backflush time (60 s).
3. Drip (or move) time (30 s).

The flow paths shown in figure ?? are representative of the flow paths during the dosing time, but the flow rates and paths change during the backflush and move time. Representative fluid flows in the system during these periods for a
scaled-down version of the production line system (3 PG dosing stages and 2 DI dosing stages), which we refer to as the mini-stack rig, are shown in figure [6.4]. Index times in this case would be 900 s for a complete extraction process.

![Mini-stack rig diagram](image)

**Figure 6.4:** Fluid flows on mini-stack rig. (a) Fluid flows during dosing time. (b) Fluid flows during backflush time. (c) Fluid flows during drip (move) time before stacks move.

An extra tank called the PG preheat tank is used to preheat the incoming PG fluid to the set point temperature. The set point temperature is the required temperature for PG entering the stacks. Where volume flow rates are indicated, these are representative flow rates during steady state operation and may vary, particularly during filling and emptying of stacks. The backflush and drip time are essentially kept constant so any change in index time will just increase or decrease the dosing time.

**Dosing time** During the dosing time, fresh PG enters the system at the top of the last PG tower (PG refresh) and flows down through the stack into the tank of the last tower. PG moves from tank to tank via a weir system at the same rate as it enters the system and leaves the system, to be disposed of, at this rate from the first tank. At each stage (except the last) PG is cycled from the tanks.
through a heater to the shower heads, down through the stack and back into the tanks at a constant rate (PG circulation). The heater operates in order to have its outlet at the target temperature. Some fluid may also be circulated through the heater and back into the tank to maintain tank temperature.

**Backflush time** At the end of dosing time, PG delivery to the stack in the last PG tower is stopped and backflush time begins. The fresh PG dose is diverted to the top of the second last stack. Similarly the flow from the tank at the bottom of the second last tower is diverted to the top of the third last tower and so on depending on the number of stacks in the system (hence back-flushing). The purpose of back-flushing is to prevent the transport of D3O against the flow of PG in the system when the stack moves to the next washing stage.

**Drip/move time** Following back-flushing, a short period of 30 s is allowed to shut off all the PG flows to the stacks, allow for any dripping from the shower-heads as they shut off and move the stacks from one position to the next. Of course a certain amount of fluid will drain from all stacks during this period leading to an increased weir flow. Similarly, when dosing restarts, fluid in the stack needs to be replenished, leading to a temporary reduction or cessation in the weir flow and a drop in tank volumes. This will be more pronounced in stage one, where a ‘dry’ stack must be filled. Tanks should have sufficient volume capacity to maintain circulation flow during this stack refilling period.

Following extraction in the PG stages, enough process aid should have been removed. Now the PG needs to be removed. To do this the lenses are washed with deionised water (DI) at a number of DI stages. They operate in the same way as the PG stages with fresh DI entering at the top of the last DI tower and being recycled through the system before draining off from the tank at the first DI tower. The DI also needs to be maintained at a given target temperature during washing although this is much lower than for PG and may be 55–65 °C. The ratio of PG extraction time to DI extraction time used is 3 : 2 as outlined above.
6.3 Key modelling questions

There are a number of interesting questions relating to the design and optimal use of the hydration process outlined above. These fall into the general categories of heat transport modelling and chemical transport modelling. These questions will be outlined and explored in the following chapters.

6.4 Experimental hydration rig and production line hydration process

For the purposes of investigating the operation of the new hydration process, Vistakon commissioned a scaled down version of its production line hydration process to conduct experiments. This scaled down process is called the mini-stack rig. Various experiments have been conducted on the mini-stack rig, collecting data such as temperature traces at different locations and final concentrations of D3O and PG in lenses, under various conditions. All experimental results presented in this thesis were obtained by other researchers on behalf of Vistakon. Process parameters that were varied included; total dosing time, refresh and circulation flow rates, index times and temperatures. This data can be used to parametrise and validate models of the mini-stack rig. Once models have been validated, parameters can be changed for the real production line hydration system. Care needs to be taken to ensure that the models properly incorporate the dependence of the particular process of interest, on the key parameters which change from the experimental rig to the production line. When particular mechanisms have to be extrapolated outside the range of experimental data, or little data exists, it is important to make conservative assumptions to ensure estimated quantities err on the side of caution. For example, when predicting heater size requirements, it is desirable to over-predict size requirement rather than under-predict. Thus wherever necessary, modelling assumptions will err on the side of safety. If greater prediction accuracy is required, further experimental data or insight may then need to be sought. In the following sections, the key features of the mini-stack rig and production line process will be described and the main physical differences outlined. The nature of experiments carried out will be described in chapters and §.
6. CONTACT LENS MANUFACTURING PROCESS

6.4.1 The mini-stack rig

The mini-stack rig system has five stages, three PG dosing stages and two DI dosing stages. Unlike the production line system, stacks must be fed manually into the system, before being mechanically conveyed through the dosing stages at the specified cycle time. Process variables, including cycle time, refresh flow rate, circulation flow rate for each stage, set point temperatures, backflush and move times can be varied as required. Each tank in the system is equipped with a heater, each of which is manufactured by Swiss company Regloplas. The mini-stack rig has six 18 kW direct heaters. Each tank have a volume of approximately 10 l and is manufactured from stainless steel. The tanks share common walls. The tanks, plumbing system and shower-heads in the mini-stack rig are not insulated. Each stage has space for one stack of thirty trays. The plumbing configuration shown in figure 6.4 is used in a number of experiments. Some experiments were also performed under a different plumbing configuration where fresh solvent was delivered to the tank in stage 3 rather than to the top of the stack.

6.4.2 The production line hydration system

The production line hydration system has ten main dosing stages. The first six are PG dosing stations and are followed by four DI dosing stages. There is also an extra stage, called the destack stage, where stacks are dismantled. There is a number of differences between the production line model and the mini-stack rig. The capacity of each tank is 301, three times that in the mini-stack rig. Each stage now has space for two stacks and so each tank feeds two shower-heads. The tank on the final PG dosing stage has been replaced with a catch-pan so that the outflow from the stacks in stage six goes directly into tank five. Similarly the tank on the final DI dosing stage (stage ten) has been replaced by a catch pan. Tank eight feeds stacks in both stages seven and eight and is equipped with two Regloplas heaters for this purpose. Tank seven is still in place, but is now only connected to the DI effluent storage and so only collects waste DI leaving the system. Tanks, plumbing and shower-heads on the production line system will also be insulated to minimise heat lost from these components. Each tank is equipped with a Regloplas heater. For safety reasons, the heaters in the production line system are indirect heaters, in contrast to the direct heaters on the mini-stack rig. This just means that the heating element is...
not in direct contact with the hydration fluid in the case of the production line whereas it is for the mini-stack rig. As a result, the heaters are less efficient on the production line system. The size of the heaters on the production line system should be determined to meet demand. Any model developed and validated for the mini-stack rig system, must be carefully adapted to take account of the different set up on the production line model before it can be used to make meaningful predictions.
CHAPTER 7
HEAT TRANSPORT IN THE CONTACT LENS HYDRATION PROCESS

7.1 Introduction

The effective operation of the hydration system outlined in chapter relies on maintaining the hydration fluids at set point temperatures. The required operating temperature for PG dosing is above 90°C. There is also a specified tolerance for deviations from the set point. The process specifications may be 96 ± 2°C. The DI dosing process requires much lower operating temperatures. The process specifications may be 55 ± 2°C or lower. In order to maintain the set point temperatures, each tank is equipped with a heater or temperature control unit supplied by Swiss company Regloplas. Hydration fluid is pumped from the tank through the heater, where it is heated to set point temperature, and delivered to the top of the stack. The heaters also allow fluid to be recirculated directly back into the tank in order to maintain tank temperature, if this is deemed necessary.

For PG dosing, an extra tank and heater is used to preheat PG to the set point temperature. The heater on the preheat tank needs to be sized to heat PG from room temperature to the set point temperature at the specified refresh flow rate into the system. The other heaters need to be sized in order to replace energy
lost in each stage. In particular the first stage is expected to require more energy in order to heat a cold incoming stack up to equilibrium temperature. It should be noted that the set point temperatures are measured at the heater outlet. The temperature in the tanks or at the bottom of the stacks may be outside the process temperature specifications. In the case of the bottom of the stack, it is of course desirable to be as close to the temperature specification as possible. The heaters use a PID (Proportional-Integral-Derivative) control system in order to maintain outlet temperature at the set point. The goal is to determine the heater sizes, so that these set points can be attained.

For DI dosing, a preheat tank is not required because deionised water can be delivered from factory supplies at temperatures of 60°C. Thus for the DI dosing system, consideration just needs to be given to recovering energy lost in each stage. In addition to this, the stack entering from the PG dosing stage is already up to temperature, and may give additional heat energy to the water as it cools to its new equilibrium temperature.

The heaters can be sourced in various sizes. They are built up in blocks of 3 kW. Thus various sizes are available (e.g. 3, 6, 9, 12, 15, 18). It should be noted that the heaters for the production line system are indirect heaters which are 90% efficient. Thus an 18 kW can deliver a maximum of 16.2 kW. The heaters on the mini-stack rig are direct heaters which are 99% efficient and so an 18 kW heater can deliver almost its full rated power. There are some practical constraints on which heater sizes can be chosen. The industry partner would like to restrict the different heater sizes to just two. This is desirable in order to limit the number of heaters that have to be held in stock to allow for replacements. It is also undesirable to have heaters which are much larger than necessary. There is insufficient space in the designed production line hydration module for an 18 kW heater on each tank, even though this would likely satisfy energy requirements. Larger heaters are also more costly to install and maintain.

7.1.1 Modelling aims

Thus the problem is to establish the minimum heater sizes (within some safety margin) that can maintain the required set point temperatures on the production line hydration system. This means heaters need to meet the steady state energy demand of the hydration system when it is in continuous operation. A second
7.2 Heat transport models

requirement is that heaters should allow for a reasonable cold start up time (i.e. heat up all tanks from cold). The specified requirement here is that heaters should allow for a start time of less than 30 minutes.

7.1.2 Modelling strategy

The hydration process described in chapter 6 is a complex process, depending on a large number of mechanisms and variables. Development of a complete, first principles, bottom up, model of all the mechanisms of heat transport in the system is impractical and almost certainly impossible to parametrise with the available data. Fortunately, the main objective is not to develop such a model. The objective here is to develop a model with sufficient resolution to predict the largest loads placed on each heater in the production line hydration system. For this purpose at least, it is more practical to develop a top-down model of the macroscale energy transfers and losses in the system and look at the energy requirements on the heaters to replace the energy losses. In this approach, we simply break the system into a number of blocks, or compartments, and model the energy losses within and transfers between models. Such a model is phenomenological, so certain model parameters will have to be fitted from experimental data. The approach here will be to start with simple energy balance compartment models, based on some simplifying assumptions, and investigate their ability to replicate experimental data collected on the mini-stack rig. Once useful models have been identified, and validated for the mini-stack rig parameters, they can be applied to the production line system. The target is to estimate the energy demands on the heaters as a function of time during one dosing cycle. The heaters should then be sized to meet these demands (plus a safety margin). Provided these estimated heater sizes deliver an acceptable start-up time and satisfy other constraints they can be fitted to the production line system.

7.2 Heat transport models

One useful way to model the transport of energy in the hydration system is to split the system into compartments and form energy balance equations for these compartments. The formulation of the model here will be outlined in the context of the mini-stack rig, but it should be clear that the model can be easily adapted
for the production line system. As previously described, the mini-stack rig has five dosing stages. Each station naturally splits into two compartments (the tank and the stack). The stack can be further divided into two compartments. One compartment consists of the fluid in the stack at any given time. The other compartment consists of the remaining thermal mass in the stack, namely the trays and the lenses and front curves. The mass of the lenses and front curves is small compared to the mass of the trays, so in practice this compartment just contains the tray material. The aim is to model energy transport within and between these compartments. There is also an extra compartment for the PG preheat tank. Thus, under this criteria, there are sixteen compartments in the mini-stack rig system. It will be assumed initially that the energy density within compartments is homogeneous, so the model will not capture spatial variations in temperature within compartments. For example, spatial variations in the temperature of the hydration fluid with vertical or horizontal position in the stack will not be captured. The assumption is by no means necessary, but results in less fitting parameters in the model. It will only be justified by the model’s ability to replicate experimental data and provide estimates of heater load with sufficient accuracy.

Under the assumption of well-mixed compartments, the compartment temperatures only depend on time. We denote the temperature in each compartment as follows:

- $T_{a,i}(t)$ is the temperature in the fluid in stage $i$ at time $t$.
- $T_{b,i}(t)$ is the temperature in the tray material in stage $i$ at time $t$.
- $T_{d,i}(t)$ is the temperature in the tank in stage $i$ at time $t$.

The index $i$ indicates the stage number, while the subscripts $a$, $b$ and $d$ denote the fluid in stack, stack material (plus front curves) and fluid in tank compartments respectively. The index for the PG preheat tank will be $i = 6$. Variables and parameters specifically relating to each compartment will use the appropriate subscript. The stack material is made from a plastic called Ultem. Parameters associated with the tray material specifically, rather than with the front curves, will use the subscript $e$. 
7.2 Heat transport models

7.2.1 Assumptions for preliminary compartment model

It is desirable to keep the compartment model as simple as possible but still capture the main energy transfers in the system. With this in mind, a number of simplifying assumptions are made. Assumptions can be relaxed or removed if deemed necessary. The initial model will just describe energy transport in the system during the dosing time. The following assumptions are made:

- As outlined above, there is no spatial variation in temperature within model compartments.

- The volume of fluid in stacks and tanks in the model is kept constant. This will be true for the majority of the dosing cycle, but some emptying and filling of stacks and tanks will take place during and following the move time. In particular the stack in stage one has to be filled from empty when it enters the system. The volume of each compartment could be modelled with a separate equation but this adds an extra layer of complexity to the model and requires specification of the time dependent fluid fluxes between compartments.

- Initially, estimates of heater loading will be made, assuming the dosing time takes up the full cycle time and disregarding changes to flow paths during backflush and drip time.

In order to simulate the moving of the stacks from stage to stage after each cycle time some further assumptions will have to be made. These will be outlined once the model for one dosing cycle has been presented.

7.2.2 Energy transport during dosing time

The flow paths between compartments during the dosing cycle are shown in figure 7.1. The change in heat energy per unit time in any compartment is simply the sum of the energy produced in the compartment and the energy entering the compartment minus the energy leaving the compartment, per unit time. The main energy sources and losses in a typical stage are shown in figure 7.2. The energy transfers represented are

- Heat energy carried in fluid flow between compartments.
Heat energy losses from plumbing between stacks or losses due to fluid evaporation are not explicitly accounted for. However, as the model parameters are being fitted to data, these losses may be incorporated into other terms. Volume loss of hydration fluid due to evaporation is also neglected.

The energy balance equations will vary from stack to stack depending on the fluid flows in a given stack and many parameters are different for each stack. The general form of the energy balance equations, accounting for the transfers in stack $i$ represented in figure 7.2 is...
7.2 Heat transport models

\[ V_a \rho_c^* \frac{dT_{a,i}}{dt} = H(T_{d,i}, i) \frac{Q_1}{Q_3 + Q_4} + Q_4 \rho_c^*(T_{d,i} - T_{a,i}) \]
\[ + h_e A_e (T_{b,i} - T_{a,i}) - h_{a,\text{air}} A_{a,\text{air}} (T_{a,i} - T_{RM}), \]  
\[ \text{(7.2.1)} \]

\[ V_e \rho_c^* \frac{dT_{b,i}}{dt} = -h_e A_e (T_{b,i} - T_{a,i}) - h_{e,\text{air}} A_{e,\text{air}} (T_{b,i} - T_{RM}), \]  
\[ \text{(7.2.2)} \]

\[ V_d \rho_c^* \frac{dT_{d,i}}{dt} = Q_1 \rho_c^*(T_{d,i+1} - T_{d,i}) + Q_4 \rho_c^*(T_{a,i} - T_{d,i}) \]
\[ + H(T_{d,i}, i) \frac{Q_3}{Q_3 + Q_4} + h_d(i) A_d(i) (T_{d,i+1} - T_{d,i}) \]
\[ - h_{d}(i - 1) A_d(i) (T_{d,i} - T_{d,i-1}) - h_{d,\text{air}} A_{d,\text{air}} (T_{d,i} - T_{RM}). \]  
\[ \text{(7.2.3)} \]

The first two equations hold for \( i = 1, 2, \ldots, 5 \) while the third holds for \( i = 1, 2, \ldots, 6 \). Equations and parameters vary depending on the stack number although this is not explicitly denoted in the equations. For example, the fluid density is different for PG and DI, so that, while the fluid density is written \( \rho \), it is equal to the density of whatever liquid is in stack \( i \). Also all terms represented in the equations are not active in some stages. Thus, we have sixteen equations for the temperature of each compartment in the system. To solve these for a given wash cycle we just need the initial temperatures at the start time in

![Figure 7.2: Energy transfers in a typical stage.](image)
7. HEAT TRANSPORT IN THE CONTACT LENS HYDRATION PROCESS

each compartment:

\[ T_{a,i}(t_{\text{start}}) = T_{a0,i}, \quad T_{b,i}(t_{\text{start}}) = T_{b0,i}, \quad T_{d,i}(t_{\text{start}}) = T_{d0,i}, \quad i = 1, 2, \ldots, 6. \]  \hfill (7.2.4)

To solve the equations over a number of wash cycles for wash time \( t_w \) one proceeds as follows:

1. Define some sensible initial conditions, e.g. all compartments at room temperature.

2. Solve the equations up to the cycle time \( t = t_w \).

3. Define new initial conditions for the next cycle, e.g. tank temperatures and fluid temperatures in stack \( i \) remain the same, but the new initial temperature of stack \( i \) is the final temperature of stack \( i - 1 \) from the previous cycle. The first stack is at room temperature.

4. Now solve for the next cycle.

5. Repeat process to solve for consecutive cycles.

6. System should reach ‘steady state’ cyclical behaviour after a number of washes. At this point system behaviour is identical from cycle to cycle so all temperature variables should have a period equal to the cycle time.

7.2.2.1 Model parameters

The parameters used, directly or indirectly, in the compartment model presented in equations (7.2.1)-(7.2.3) are listed in table 7.1.

7.2.3 Heat transfers and losses in the compartment model

The compartment model accounts for a number of heat transfers and losses as shown in figure 7.2. The modelling of these transfers will be discussed in the following sections.
7.2 Heat transport models

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_a(i)$</td>
<td>volume of the fluid in stack $i$.</td>
</tr>
<tr>
<td>$V_b(i)$</td>
<td>volume of the lenses in stack $i$.</td>
</tr>
<tr>
<td>$V_c(i)$</td>
<td>volume of the stack (tray material) in stack $i$ (this may also include the lens volume).</td>
</tr>
<tr>
<td>$V_d(i)$</td>
<td>volume of the tank in stack $i$.</td>
</tr>
<tr>
<td>$\rho(i)$</td>
<td>density of fluid in stack $i$.</td>
</tr>
<tr>
<td>$\rho_p$</td>
<td>density of PG.</td>
</tr>
<tr>
<td>$\rho_w$</td>
<td>density of DI.</td>
</tr>
<tr>
<td>$\rho_e$</td>
<td>density of stack material.</td>
</tr>
<tr>
<td>$c^*(i)$</td>
<td>specific heat capacity of fluid in stack $i$.</td>
</tr>
<tr>
<td>$c_p$</td>
<td>specific heat capacity of PG.</td>
</tr>
<tr>
<td>$c_w$</td>
<td>specific heat capacity of DI.</td>
</tr>
<tr>
<td>$c_e^*$</td>
<td>specific heat capacity of stack material.</td>
</tr>
<tr>
<td>$t_w$</td>
<td>cycle (wash) time at one station.</td>
</tr>
<tr>
<td>$A_d(i)$</td>
<td>Cross-sectional area between tank $i$ and tank $i + 1$.</td>
</tr>
<tr>
<td>$A_{d,\text{air}}(i)$</td>
<td>Area of wall in tank $i$ exposed to air.</td>
</tr>
<tr>
<td>$A_e(i)$</td>
<td>Contact area between fluid and trays in stack $i$.</td>
</tr>
<tr>
<td>$A_{e,\text{air}}(i)$</td>
<td>Contact area between stack $i$ and surrounding air.</td>
</tr>
<tr>
<td>$A_{a,\text{air}}(i)$</td>
<td>Contact area between fluid and air in stack $i$.</td>
</tr>
<tr>
<td>$h_d(i)$</td>
<td>Heat transfer coefficient between tank $i$ and tank $i + 1$.</td>
</tr>
<tr>
<td>$h_{d,\text{air}}(i)$</td>
<td>Heat transfer coefficient between tank $i$ and surrounding air.</td>
</tr>
<tr>
<td>$h_e(i)$</td>
<td>Heat transfer coefficient between fluid and stack material in stack $i$.</td>
</tr>
<tr>
<td>$h_{e,\text{air}}(i)$</td>
<td>Heat transfer coefficient between stack $i$ and surrounding air.</td>
</tr>
<tr>
<td>$h_{a,\text{air}}(i)$</td>
<td>Heat transfer coefficient between fluid and air in stack $i$.</td>
</tr>
<tr>
<td>$Q_1$</td>
<td>volume flow rate of liquid between from tank to tank.</td>
</tr>
<tr>
<td>$Q_2$</td>
<td>volume flow rate from tank to heater.</td>
</tr>
<tr>
<td>$Q_3$</td>
<td>volume flow rate being circulated through heater back into tank.</td>
</tr>
<tr>
<td>$Q_4$</td>
<td>volume flow rate from tank to stack (through heater) and back to tank.</td>
</tr>
<tr>
<td>$T_{RM}$</td>
<td>room temperature (temperature of surrounding air).</td>
</tr>
<tr>
<td>$T_1$</td>
<td>target temperature for heaters in PG stacks.</td>
</tr>
<tr>
<td>$T_2$</td>
<td>target temperature for heaters in DI stacks.</td>
</tr>
<tr>
<td>$H(T_{d,i}, i)$</td>
<td>this function gives the heater output based on the inlet (tank) temperature to fix the outlet temperature.</td>
</tr>
</tbody>
</table>

Table 7.1: Parameters for heat transport compartment model.
7. HEAT TRANSPORT IN THE CONTACT LENS HYDRATION PROCESS

7.2.3.1 Heat transfer in fluid flow

Heat energy transfers from compartment to compartment in the fluid through advection. For example, the fluid flow rate $Q_1$ from tank $i+1$, which is at temperature $T_{d,i+1}$, to tank $i$ carries the following heat flow ($J/s^{-1}$):

$$q_1 = Q_1 \rho c^* T_{d,i+1}. \quad (7.2.5)$$

Thus the heat flow is simply

$$\text{volume flow rate} \times \text{fluid density} \times \text{specific heat capacity} \times \text{temperature in compartment fluid came from.} \quad (7.2.6)$$

7.2.3.2 Heat transfer from tank to tank through common wall

The fluid in adjacent tanks share the same wall and so heat is transferred through the wall via conduction. The heat flow is modelled by the following expression

$$h_d(i) A_d(i) (T_{d,i+1} - T_{d,i}). \quad (7.2.7)$$

The heat flow is proportional to the area of the common tank wall and the difference in temperature of the fluids on either side. The constant of proportionality is the heat transfer coefficient and will vary depending on the fluids on either side. This constant accounts for the resistance to heat flow in the stainless steel wall and the fluids on either side. We can calculate it by finding the total resistance to flow of the fluid-wall-fluid interface. The heat transfer coefficient of the wall is easy to calculate. It is simply the ratio of the thermal conductivity $k_d$ of stainless steel to the thickness of the wall $s_d$. The transfer coefficients of the liquids are much harder to estimate without experiment. We estimate them as the thermal conductivity of the liquid $k_{f,i}$ (f represents either PG or DI), divided by some length scale $l_d$, which we can only guess without experimental insight. This length scale will be the fitting parameter for this term from available experimental data. The total transfer coefficient is the reciprocal of the total thermal resistance given by:

$$h_d(i) = \frac{1}{l_d/k_{f,i} + s_d/k_d + l_d/k_{f,i+1}}. \quad (7.2.8)$$
7.2.3.3 Other heat transfers through common interfaces

Heat energy transfers between compartments and the surrounding atmosphere are all modelled by equations that have the same form as (7.2.7). Once the interface area is known, the difficulty lies in estimating a suitable heat transfer coefficient. In all cases the transfer coefficient is estimated by dividing the thermal conductivity of the medium with a suitable length scale \( l \).

7.2.3.4 Ideal heater operation

The heaters in each stack should operate to keep the heater outlet at a target temperature \( T_{\text{target}} \). We denote the heater output at time \( t \) by \( W_{\text{heater}}(t) \). Fluid flows into the heater at a rate \( Q_2 \text{ m}^3\text{s}^{-1} \). The energy balance for a heater at time \( t \) is

\[
W_{\text{heater}}(t) = Q_2 \rho c^*(T_{\text{outlet}}(t) - T_{\text{inlet}}(t)).
\] (7.2.9)

For heater \( i \), the inlet temperature is the temperature in tank \( i \), \( T_{d,i}(t) \). We simply choose the wattage to ensure \( T_{\text{outlet}}(t) = T_{\text{target}} \). This is only possible for a range of temperatures. If the tank temperature is greater than the target temperature we would need to take out energy, which the heater can’t do, so we just turn it off. Also if the inlet temperature is too low the heater may not be powerful enough to get the required temperature rise. For example we have

\[
T_{\text{outlet}}(t) = T_{\text{inlet}}(t) + \frac{W_{\text{heater}}(t)}{Q_2 \rho c^*}.
\] (7.2.10)

The maximum temperature that can be added for a 18 kW heater with a volume flowing in of 301 min\(^{-1}\) with the appropriate densities and specific heat capacities for PG is approximately 12°C. If the tank temperature is more than 12°C below target, the target temperature cannot be reached and the heater should operate at maximum output. Thus heater demand \( W_i(t) \) for heater \( i \) in our system would be

\[
W_i(t) = Q_2(i) \rho(i) c^*(i)(T_{\text{target},i} - T_{d,i}(t)).
\] (7.2.11)
Heater output for a heater in stack $i$, with wattage $W_{\text{max},i}$ would be controlled as follows:

$$W_{\text{heater},i}(t) = \begin{cases} 
0, & \text{if } W_i(t) < 0, \\
W_i(t), & \text{if } 0 \leq W_i(t) \leq W_{\text{max},i}, \\
W_{\text{max},i}, & \text{if } W_i(t) > W_{\text{max},i}. 
\end{cases} \quad (7.2.12)$$

We can use $H(T_d,i,i) = W_{\text{heater},i}(t)$ to model the instantaneous heater demand in the compartmental model. In practice, the idealised heater operation described here is not possible and heater operation is controlled using a PID (Proportional-Integral-Derivative) controller. The PID controller operates to maintain the heater outlet temperature at a defined set point. The tuning of a PID controller is a difficult problem and has been a major area of research since Ziegler and Nichols \cite{76} presented their tuning methods in 1942 \cite{5}. PID operation and tuning is a little outside the scope of the work here, but as operation of heaters during experiments is determined by PID control, incorporation of PID control into the model may be necessary to replicate observed results. For this reason, modelling a PID controller will be discussed in the next section. In general, the idealised heater operation term will be used to estimate heater demand for steady state periodic heater operation. In this situation, a properly tuned PID controller should closely replicate the idealised behaviour. For experimental situations where system loads are being varied to test different situations the response generated by the PID controller will need to be modelled to capture the observed behaviour.

### 7.2.3.5 PID controlled heater

In this section, an overview of the main elements of a PID (Proportional-Integral-Derivative) controller will be presented. The presentation will be brief, so the interested reader should refer to a standard reference on feedback control, such as ref. \cite{6}, for a complete description. In the hydration system, heater operation is controlled by PID controllers. This is not surprising as over 95% of all industrial control problems are solved by PID controllers \cite{6}. The heaters are controlled to maintain the heater outlet temperature at a set point. In general, the set point may be a function of time so it is denoted as $r(t)$. The process variable is the quantity to be controlled, in this case the outlet temperature. It is denoted as $y(t)$. The current value of the process variable and the set point are used
7.2 Heat transport models

determine the error, or deviation from the set point, \( e(t) \). The error is given by:

\[
e(t) = r(t) - y(t).
\]  
(7.2.13)

The current error and previous errors are used to calculate the control output \( u(t) \). The control output of a PID controller is given by:

\[
u(t) = K_p e(t) + K_i \int_0^t e(\tau) d\tau + K_d \frac{de(t)}{dt}.
\]  
(7.2.14)

where \( K_p \) is the proportional gain, \( K_i \) is the integral gain and \( K_d \) is the derivative gain. The control output is often written as:

\[
u(t) = K_p \left( e(t) + \frac{1}{T_i} \int_0^t e(\tau) d\tau + T_d \frac{de(t)}{dt} \right),
\]  
(7.2.15)

where \( T_i \) is the integral time and \( T_d \) is the derivative time. The control output is the sum of proportional, integral and derivative terms. These terms can be thought of as adjusting the output for present, past and predicted future error respectively. The control output signal is sent to the control element (in this case the heater) causing it to change its output. The objective is to attain \( e(t) = 0 \).

The signal may need to scaled before being implemented by the heater but, allowing for this, the controller should give a signal to the heater to run somewhere between its minimum and maximum output. The first term in the control output is the proportional term. For a P only controller, the control signal (ignoring scaling) is given by

\[
u(t) = \begin{cases} u_{\text{min}}, & \text{if } e(t) \leq e_{\text{min}}, \\ K_p e(t), & \text{if } e_{\text{min}} < e(t) < e_{\text{max}}, \\ u_{\text{max}}, & \text{if } e(t) \geq e_{\text{max}}. \end{cases}
\]  
(7.2.16)

where \( u_{\text{min}} \) and \( u_{\text{max}} \) are the minimum and maximum control signals corresponding to the minimum and maximum errors, \( e_{\text{min}} \) and \( e_{\text{max}} \), between which the proportional control is active. Below the minimum error the control signal is at its minimum and above the maximum error the control signal is maximum. For a heater, this means that when the error is zero or less the heater is turned off \( (u_{\text{min}}) \), while, when the error is large enough, the set point cannot be reached and the heater is at its maximum setting \( (u_{\text{max}}) \). In between these bands is the
proportional band, given by \((e_{\text{min}}, e_{\text{max}})\) or \((\frac{u_{\text{min}}}{K_p}, \frac{u_{\text{max}}}{K_p})\). In this error range, the control signal is a linear function of the error. As the ideal proportional gain of a system can change over time, proportional controllers have the drawback that the steady state error value is often different from \(e(t) = 0\).

To eliminate steady state error, the integral term is included, resulting in a PI controller. The integral term sums up past errors and adjusts the control output accordingly to eliminate steady state error, ensuring \(e(t) = 0\) at steady state, provided a steady state exists. One issue with the integral term is that of integral windup [6]. This happens when the control element is unable drive the system to its set point for a period of time, due to system disturbances outside its normal operation. The set point error during this period leads to a large integral term so that when disturbances are removed, the control signal remains very high or low for a period of time. Thus the integral term can lead to a slow transition back to normal operation as it ‘unwinds’. This may also be an issue, for example, when heating hydration fluid from room temperature. If the set point cannot be reached, errors will accumulate in the integral term and cause an overshoot in temperature after the set point is reached. The integral term continues to drive the heating above the set point in this case.

Finally the derivative term is applied to predict future error, by using a linear extrapolation of the current rate of change of error, \(T_d\) time units into the future. The derivative term can help to avoid set point overshoot. The derivative term is rarely used in practice as it is very sensitive to noise in the measurement of the process variable. For this reason it will not be discussed further here.

On the Regloplas heaters, the control signal is delivered as a percentage of the heater’s total output. The control signal \(CO(t)\) can be written as:

\[
CO(t) = \left( \frac{100}{P_{\text{band}}} \right) \left( e(t) + \frac{1}{T_i} \int_0^t e(\tau)d\tau \right),
\]

where \(P_{\text{band}}\) is the width of the proportional heating band below the set point. The proportional gain is given by \(K_p = \frac{W_{\text{max}}}{P_{\text{band}}}\). An example of the control signal generated from the proportional part of a PI controller on a Regloplas heater is shown in figure 7.3. Accumulation of errors in the integral term, resulting from prolonged periods the process variable is above or below the set point temperature, due to a system disturbance, can lead to control signals significantly above 100% or below 0%. For signals above 100% the heater runs at maximum capacity.
and shuts off for signals below 0%. Thus when heater action is modelled by PI control the wattage delivered by heater $i$, $W_{\text{heater},i}(t)$, is given by

$$W_{\text{heater},i}(t) = \begin{cases} 
0, & \text{if } CO(t) < 0 \\
W_{\text{max},i}, & \text{if } CO(t) > 100 \\
\left(\frac{CO(t)}{100}\right)W_{\text{max},i}, & \text{if } 0 \leq CO(t) \leq 100
\end{cases} \quad (7.2.18)$$

Note that the heater action, $H(T_{d,i},i)$, no longer depends explicitly on the tank temperature $T_{d,i}$ in this case.

A problem arises when a disturbance as described above is removed, the set point temperature can now be attained, but the integral term is still compensating for the past errors. As discussed above this is called integral windup and contributes to a slow transition back to normal operation. There are a number of methods to avoid windup, but it is not known what methods, if any, are applied in the Regloplas heaters. When attempting to replicate heater behaviour from experiments, it must be taken into account that anti-windup methods may be used by the heaters. When sizing the heaters for the production line, potential PID control issues will not be considered. It will be assumed that the heaters can be tuned to closely replicate the ideal heater operation outlined in section 7.2.3.4.
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7.2.4 Cycle averaged heat transport model

The compartment models outlined above attempt to estimate the energy demands placed on system heaters during a dosing cycle. An alternative approach is to estimate the average demand placed on the heaters during a cycle. This should provide a quicker solution and also provide a reference with which to compare results from the time-dependent model.

During steady state operation the heaters simply need to replace the heat losses in the system. Thus the heater demand can be estimated by just considering the heat losses from the system and not all the heat transfers in the system. To do this it is assumed that all compartments are at the target temperatures for the hydration fluid in that stage. So compartments in PG stages and the PG preheat tank are at temperature $T_1$. Compartments in DI stages are at temperature $T_2$. The average heater demand in a given wash cycle is then considered, assuming all compartments are at target temperatures. Each heater needs to provide enough heat energy during the wash cycle to balance the losses. Besides the heat losses to the surrounding atmosphere the following are also accounted for:

1. Heater 1 needs to provide enough heat energy to heat a cold stack to target temperature during the dosing cycle. This is assumed to happen in one stage.

2. The PG pre-heat tank heater needs to provide enough heat energy to heat the PG entering the system from room temperature to the target temperature.

3. Heaters on PG tanks adjacent to DI tanks will have to provide heat energy to compensate for the loss of heat through the tank wall.

4. Heaters on DI tanks adjacent to PG tanks will have to provide less heat energy due the gain of heat through the tank wall.

5. The first DI stage will receive heat energy from the stack as it reduces in temperature from $T_1$ to $T_2$. This is assumed to happen in one stage.
For the mini-stack test rig we have the following equations for heater demand:

\[ H_{av,1} = \frac{\rho_e V_e c_e^*}{t_w} (T_1 - T_{RM}) \]
\[ + (h_{e,\text{air}} A_{e,\text{air}} + h_{d,\text{air}} A_{d,\text{air}} + h_{a,\text{air}} A_{a,\text{air}})(T_1 - T_{RM}), \]
\[ (7.2.19) \]

\[ H_{av,2} = (h_{e,\text{air}} A_{e,\text{air}} + h_{d,\text{air}} A_{d,\text{air}} + h_{a,\text{air}} A_{a,\text{air}})(T_1 - T_{RM}), \]
\[ (7.2.20) \]

\[ H_{av,3} = (h_{e,\text{air}} A_{e,\text{air}} + h_{d,\text{air}} A_{d,\text{air}} + h_{a,\text{air}} A_{a,\text{air}})(T_1 - T_{RM}) \]
\[ + h_d(3) A_d(3)(T_1 - T_2), \]
\[ (7.2.21) \]

\[ H_{av,4} = (h_{e,\text{air}} A_{e,\text{air}} + h_{d,\text{air}} A_{d,\text{air}} + h_{a,\text{air}} A_{a,\text{air}})(T_2 - T_{RM}) \]
\[ + h_d(3) A_d(3)(T_2 - T_1) + \frac{\rho_e V_e c_e^*}{t_w} (T_2 - T_1), \]
\[ (7.2.22) \]

\[ H_{av,5} = (h_{e,\text{air}} A_{e,\text{air}} + h_{d,\text{air}} A_{d,\text{air}} + h_{a,\text{air}} A_{a,\text{air}})(T_2 - T_{RM}) \]
\[ + h_d(5) A_d(5)(T_2 - T_1), \]
\[ (7.2.23) \]

\[ H_{av,6} = (h_{d,\text{air}} A_{d,\text{air}} + Q_1 \rho_p c_p^*)(T_1 - T_{RM}) + h_d(5) A_d(5)(T_1 - T_2), \]
\[ (7.2.24) \]

where \( H_{av,i} \) gives the cycle averaged heater demand in stage \( i \). Although it is not explicitly denoted, some parameters will depend on stage number. These equations can be obtained by substituting the target temperatures into the compartment model, adding the equations for each compartment and integrating over the wash cycle. Extra terms just need to be added for the changing of the steady state temperature of the stack in stages 1 and 4. The output is an estimate of average heater demand for each heater over a dosing cycle.

### 7.2.5 Higher resolution heat transport models

The compartment models introduced in the previous sections make no attempt at modelling spatial variation of temperatures within compartments. It is relatively easy to extend these models to include spatial variation within compartments without introducing the complex geometries of the compartments. For example, a natural extension would be to let the temperature of fluid within a stack depend on the vertical position within a stack by introducing a coordinate for vertical position in a stack. However the primary interest here is to produce estimates of the energy demands on the heaters, not determining the temperature distribution in the stack. If reasonable estimates can be produced with the simpler model, there is little to be gained from introducing more complexity and extra terms to
be parametrised into the model. For this reason, more complex models of heat transfer will not be pursued here.

7.3 Mini-stack rig experiments

Due to the time and effort required to collect data from the mini-stack rig, there is a limited set of experimental data. The experiments break into two types:

- The majority of experiments conducted to investigate heat transfer in the mini-stack rig only used deionised water in the system. Thus all five stages in these experiments ran with DI. Some of these DI experiments also investigated heat loss from a single stack.

- Only one experiment was conducted in which the first three stages ran PG and the final two stages ran DI as intended. Part of the reason for this is safety issues involved with heating PG to high temperatures with direct heaters, such as those in the mini-stack rig.

The experiments each have some drawbacks, which make it more difficult to use them to fit and validate models. These drawbacks will be outlined during the description of the experiments.

7.3.1 Mini-stack experiments with DI water

The mini-stack rig system was run through a number of washing cycles with all stages running deionised water. The system was loaded with stacks of thirty trays, but only the top four trays had front curves in place. The set point temperatures for the first three stages were 95°C, closely corresponding to the required processing temperature for these stages when running PG hydration fluid. The set point temperature for the final two stages was 65°C again typical of processing conditions for DI stages on the production line. The main system parameters are listed in table 7.2. The listed flow rates are the flow rates to shower heads in each stage during dosing. DI was recirculated through the heaters directly back into the tanks at 30 l min⁻¹ to maintain tank temperatures. The shower head in stage five is fed directly with DI at 40°C. In place of PG, DI was pumped to the top of stage three from a 200 l barrel at 41 min⁻¹. The temperature in the barrel was approximately 25°C.
The other key points of the experiment are as follows:

- Initially the tanks were full of DI at room temperature, taken to be 23 °C.
- Five stacks were in place initially, all at room temperature.
- The tanks were heated from cold to their set point temperatures initially before dosing began.
- Once all tanks had reached set point temperatures, the system was run through four dosing cycles.
- After this, the dosing was stopped and system was left with water just recirculating for approximately 20 min.
- Following this, another four dosing cycles were completed before the experiment was complete.
- The heater outlet temperature and power output for each Regloplas heater was logged every 10 s.
- Power output was given as a percentage of heater wattage and varied from −100% to 100%. However, as cooling was not enabled on the Regloplas temperature control units, only readings from 0% to 100% result in heater action.
- Back-flushing only occurred in stages 1 and 2. Dosing to stages 3 and 5 shut off during the backflush period as expected, but the expected back-flushing in stage 4 did not occur in this experiment.
7. HEAT TRANSPORT IN THE CONTACT LENS HYDRATION PROCESS

7.3.1.1 Experimental observations

Plots of the heater outlet temperatures and power outputs during the experiments are shown in figure 7.4. It was observed that it took approximately 3 min for the tanks 4 and 5 to reach set point temperature. Tanks 1, 2, 3 and 6 took 5–6 minutes to reach their set point temperatures. In the stages with a set point of 95°C, the power output of the heaters remains at 100% for about 2 min initially. At this point the temperatures enter the proportional heating band, which is 16°C below the set point, and power output decreases linearly as temperature approaches the set point.

Following this the system runs through four cycles, which can be seen clearly in some of power output curves in figure 7.4. It can be seen that heater 2 reaches a relatively steady power output, while other heaters display more of a cyclical behaviour. This is due to the fact that stage 2 receives relatively few disturbances to change its heater loading. The stack has already been heated from cold in stage 1 and dosing continues for most of the cycle time in stage 2. In contrast, in stage 1, the PI controller has to respond to the new demand of a cold stack entering in each cycle. In stage 3, the PI controller has to respond to the shutting off of incoming DI during backflush and move time, which reduces its demand during this period. This response of the PI controller to disturbances, also leads to a more variable outlet temperature in stages 1 and 3 compared to stage 2. It can be seen that after the first couple of cycles the heaters start to approach a steady cyclic behaviour, with the exception perhaps of heater 4.

Table 7.3 shows the mean, standard deviation, minimum and maximum values for the heater outlet temperatures and power outputs over the third and fourth cycles. As expected, heater 2 is by far the least variable in its outputs, having relatively few disturbances in load over a dosing cycle. It is notable that all of the heaters except heater 6 are operating at less than 30% of their capacity at all times. Thus reducing outlet temperature variability is a matter for PI controller tuning and not a matter of limited heater capacity. It is noted that heater 4 is never engaged and the average signal is −7.01%. It is clear that tank 4 is being overheated by conduction through its common wall with tank 3 (which is at approximately 95°C). Effectively heater 3 is taking the load of heating tank 4 as well as tank 3. This suggests that, where common walls exist between PG and DI tanks on the production line design, they should be insulated. Finally the
large difference between the minimum and maximum outlet temperature values
on heater 6 would be a cause for concern on the production line where outlet temperatures need to remain within a small tolerance of the set point. Although heater demand is at times near capacity, the actual variation in temperature arises from a control issue. When the system changes from backflush to move time, the load on the heater goes from heating 41 min\(^{-1}\) of DI from room temperature to 95 °C to just recovering energy losses from tank surfaces during move time. The integral term in the PI controller adapts to changing of system loads but errors need to accumulate over time for behaviour to change. Thus initially when system changes from backflush to move time, the heater is still providing enough energy to heat incoming DI and the outlet temperature overshoots close to 100 °C, before the integral term can compensate for errors. This can be clearly seen in figure 7.4f where the power output is dropping but the outlet temperature is spiking. Similarly when dosing is turned back on, outlet temperature will drop below set point before integral term can compensate for errors and provide for the increased load. These control issues can be solved by smarter control elements which can account for the changing loads during dosing cycles.

After the first four cycles, dosing is shut off and the DI is just left to circulate through the heaters for approximately 20 minutes. This can be seen in figure 7.4 where heater demands level off during this period. The main energy losses in the system during this period should be from the tanks’ surfaces. Thus this data should allow the heat transfer coefficients governing energy losses from the sur-
faces of tanks and transfers between tanks to be estimated. Heaters 1–3 behaved as expected during this period, adjusting to the lower demand and attaining set point temperature. The power output signal on heaters 4 and 5 decreased to −100%, showing the heating through tank walls from adjacent tanks 3 and 6 provide more than enough energy to heat tanks. Tank temperature increases well above set point and accumulated errors in the integral term drive the signal to its limit at −100%. The reduced load on heater 6 sees outlet temperature spike to over 103°C before the integral term adapts the control signal to the new demand level.

Following the idle phase, dosing was switched on and ran for four cycles. Most heaters can be seen to return to normal operation within a couple of cycles. However, the heater 5 outlet temperature drops as low as 50°C before power output increases above 0%. Heater 4 power output stays at −100% until the end of experiment despite the outlet temperature reaching as low as 59°C. It appears the accumulated errors in the integral term during the temperature overshoot in the idle phase result in a very slow transition back to normal behaviour during dosing.

The undesirable PI controller behaviour during the experiment is a concern. To confirm the explanations proposed above and validate the PI controller model proposed in section 7.2.3.5 it is useful to attempt to recreate the control signals observed in the experiment.

### 7.3.1.2 PI controller simulations

It is clear that the PI controllers’ response is sensitive to the exact heater outlet temperature trace in the experiments. There is little point in trying to replicate controller behaviour using the compartment model of the system, which is missing some of the key disturbances which drive controlled behaviour. In order to validate the model of the PI controller described in section 7.2.3.5 it is simplest to take the output temperature trace data and simulate the PI control signal. If the simulated control signal agrees with the experiment power output trace, then the PI control model is validated. Inspection of the integral and proportional terms can then be used to understand controller behaviour.

The PI controllers in question have variable settings for the proportional heating band $P_{\text{band}}$, integral time $T_i$ and derivative time $T_d$. The settings used in experiments were $P_{\text{band}} = 16°C$, $T_i = 300$s and $T_d = 0$s. Thus the derivative
The control output in equation (7.2.17) is a continuous time output. To implement on a computer we just partition the time domain into discrete intervals (10 s in this case), and discretise the integral term. Writing the proportional and integral terms as $P(t)$ and $I(t)$ we have the $CO(t) = P(t) + I(t)$. It is observed that to match initial controller behaviour it is necessary to have integral term turned off when control signal is greater than or equal to 100%. Thus the integral term does not update when $CO(t) \geq 100\%$. As control signal does not reach 100% for the rest of the experiment it is not clear if this anti windup feature holds in general, we assume here it does. The opposite does not hold. The integral term continues to update when control signal $CO(t) \leq -100\%$ to match data. The control algorithm proceeds as follows:

1. At time step $t_0$: Initialise control output $CO(t) = 100$ as tanks are heating from room temperature. Set integral term $I(t) = 0$.

2. At time step $t_k$: Calculate error from set point temperature $e(t_k) = r(t_k) - y(t_k)$. Compute proportional term:

$$P(t_k) = \frac{100}{P_{band}} e(t_k). \tag{7.3.1}$$

Update integral term if controller output is less than 100 using

$$I(t_k) = I(t_{k-1}) + \frac{100}{P_{band}T_i} e(t_k)(t_k - t_{k-1}). \tag{7.3.2}$$

Otherwise $I(t_k) = I(t_{k-1})$. Compute control output using

$$CO(t_k) = P(t_k) + I(t_k). \tag{7.3.3}$$

Note the power output $PO(t)$ recorded in experiments is between $-100$ and
7.3 Mini-stack rig experiments

100. To get this from the control output we simply apply

\[
PO(t_k) = \begin{cases} 
-100, & \text{if } CO(t) < -100, \\
CO(t), & \text{if } -100 \leq CO(t) \leq 100, \\
100, & \text{if } CO(t) > 100.
\end{cases}
\] (7.3.4)

3. Continue to repeat step 2.

![Plots of the simulated power output and actual power output data for heaters 1 and 5.](image)

**Figure 7.5:** Comparison between measured power output data and simulated power output (PI model) for (a) heater 1 and (b) heater 5.

Plots of the simulated power output and actual power output data are shown for heaters 1 and 5 in figure 7.5. It can be seen that the simulated behaviour closely matches the actual power output data. The agreement disimproves with increasing time showing a shift in the simulated output compared to actual output. This is likely due to errors in calculation of the integral term which will amplify over time. This may be down to the 10 s update time. Apart from this the simulation captures the controller response well. In particular it captures the unusual behaviour in heater 5 during the idle phase of the experiments very well.

The PI controller simulation can be used to investigate the causes of temperature variability in the system. Here we consider the fluctuations in outlet temperature in heater 5 during back-flushing and drip time and in heater 6 (pre-heat tank) during drip time. Figure 7.6 shows the PI controller signal \( CO(t) \) and its proportional and integral components, \( P(t) \) and \( I(t) \), and the corresponding temperature profile in heater 5. The period when the system enters backflush
7. HEAT TRANSPORT IN THE CONTACT LENS HYDRATION PROCESS

and drip time (105 s) is highlighted. As back-flushing begins, dosing to stage 5 stops and the load on the heater soon drops because DI at approx 40 °C is no longer entering the tank. During this period DI is just circulating through heater 5 and back into the tank. However, as can be seen in the figure, the heater is relying primarily on the integral term to drive heating during the dosing cycle. The integral term is slow to change having a large integral time $T_i$. Thus the control output remains the same and the temperature has to spike significantly to dissipate the integral term and also use the proportional term to reduce the output until the integral term can eliminate the steady state error. As the back-flush time is relatively short the system does not have time to adapt to the new energy demands and so when dosing resumes the temperature is still rising and power output dropping. As dosing begins, the energy demand is again increased and so temperature begins to drop and power output increases, due to changes in the proportional term.

Figure 7.7 shows the PI controller signal $CO(t)$, its proportional and integral components, $P(t)$ and $I(t)$, and the corresponding temperature profile in heater 6. A rapid change in behaviour can be seen during the drip time (15 s) part.
of the cycle. The temperature spikes sharply during this period. The load on the heater drops dramatically as dosing from the preheat tank is switched off, and it no longer has to heat \(41\text{ min}^{-1}\) from room temperature to set point. The controller only responds to changes in the outlet temperature and, as the integral term changes slowly, the controller continues delivering the same output causing a spike in temperature. The proportional term drops accordingly, but the integral term is very large so temperature continues to spike and is only stopped by starting of the dosing cycle and restoration of the load.

![Figure 7.7: Control output and temperature for heater 6 over a dosing cycle. The proportional \((P(t))\) and integral \((I(t))\) parts of the control output signal are also plotted.](image)

Figure 7.8 compares the simulated control signals for heaters 4 and 5 with the simulated power outputs and the actual experimental power outputs. It can be seen that the control signal drops down below \(-250\%\) for both heaters due to an extended period above set point. Errors accumulate in the integral term and thus when dosing resumes heater 4 does not reactivate within 4 cycles while heater 5 takes 2 cycles to reactivate. This is despite the outlet temperature dropping below the set point in both heaters as discussed earlier. This is a clear example of integral windup.
Figure 7.8: Comparison of the controller output signal $CO(t)$, the power output signal $PO(t)$ and the actual power output from experiments for (a) heater 4 and (b) heater 5.

The PI controller simulation verifies that the model used here can replicate controller behaviour. This is useful as it allows comparison of PI controller behaviour and the ideal heater behaviour. For example, although tank temperatures were not measured in this experiment, given the outlet temperatures and power output it is possible to reverse engineer the actual tank temperature (or at least the heater inlet temperature). Given this we can compute the ideal heater power output to achieve the set point and compare with the PI controller output. The analysis also flags some potential problems with the PI control operation. A ‘smarter’ system where the controller is aware of heater load changes over different parts of the dosing cycle and resets the integral accordingly may be necessary to minimise outlet temperature variations. Such solutions should be available from heater manufacturers or in the extensive literature on PID control.

### 7.3.1.3 Heat losses and transfers from mini-stack rig tanks

During the idle phase of the experiment, DI is just being recirculated through the heaters and back into the tanks. The main heat losses from the system will be from the surfaces of the tanks. Other losses which may occur from the system plumbing surfaces will be incorporated in the tank heat transfer coefficients. Transfers of heat energy between tanks will also occur during this period through their common walls. During this recirculation period the outlet temperatures and heater actions are steady in most tanks. Where temperature variation does occur
the overall loss or gain of temperature is small. By applying an energy balance to each tank over this period it is possible to fit the heat transfer coefficients for the tank walls in contact with air and the common tank walls. The recirculation period from 3100 s to 3300 s is considered here. The heater outlet temperatures and power output have been logged every 10 s over this period and are shown in figure 7.9. The actual tank temperature can be worked out by rearranging equation (7.2.10) to get:

\[ T_{\text{inlet}}(t) = T_{\text{outlet}}(t) - \frac{W_{\text{heater}}(t)}{Q_2 \rho c^*}. \] (7.3.5)

![Figure 7.9:](a) Heater outlet temperatures during the idle phase of the experiment. Note temperatures in heaters 1–3 are steady, temperatures in heaters 4 and 5 are increasing slowly and the temperature in heater 6 is dropping slowly. (b) Power output from heaters during the idle phase of the experiment. Note power output signal for heaters 4 and 5 was negative so power output is zero. Also output is only given in 1% increments and logged every 10 s, hence the jumps evident in heaters 3 and 6.

Outlet temperature \((T_{\text{outlet}}(t))\), wattage delivered by heater \((W_{\text{heater}}(t))\), flow rate through heater \((Q_2)\), water density \((\rho_w)\) and specific heat capacity \((c^*_w)\) are all known so we can work out the heater inlet temperature \((T_{\text{inlet}}(t))\) in each tank. A model similar to the cycle averaged heat transport model in section 7.2.4 can be used to fit the heat transfer coefficients. The main differences here are that the energy losses from stack and demands for heating stacks drop out of the model and the averaging period is 200 s. Also there is a small variation in temperature (in tanks 4–6) so the average temperature is adopted here as the
tank temperature. The energy lost or gained through the change in temperature
$\Delta T_{d,i}$ in tank $i$ over the 200 s period is added to the energy balance equations
for these tanks. All tanks contain water in this experiment so the common walls
should have the same heat transfer coefficient, which we denote as $h_d$. The heat
transfer coefficient for the tank walls to the surrounding air is denoted by $h_{d,\text{air}}$
and again should be the same for all tanks. Thus the heat balance equations are

\[
H_{\text{av},1} = h_{d,\text{air}} A_{d,\text{air}} (T_d(1) - T_{RM}) + h_d A_d (T_d(1) - T_d(2)),
\]
\[
H_{\text{av},2} = h_{d,\text{air}} A_{d,\text{air}} (2)(T_d(2) - T_{RM}) + h_d A_d (T_d(2) - T_d(1))
+ h_d A_d (2)(T_d(2) - T_d(3)),
\]
\[
H_{\text{av},3} = h_{d,\text{air}} A_{d,\text{air}} (3)(T_d(3) - T_{RM}) + h_d A_d (2)(T_d(3) - T_d(2))
+ h_d A_d (3)(T_d(3) - T_d(4)),
\]
\[
H_{\text{av},4} = h_{d,\text{air}} A_{d,\text{air}} (4)(T_d(4) - T_{RM}) + h_d A_d (3)(T_d(4) - T_d(3))
+ h_d A_d (4)(T_d(4) - T_d(5)) - \frac{\rho_w V_d c^*_w}{200} (\Delta T_{d,4}),
\]
\[
H_{\text{av},5} = h_{d,\text{air}} A_{d,\text{air}} (5)(T_d(5) - T_{RM}) + h_d A_d (4)(T_d(5) - T_d(4))
+ h_d A_d (5)(T_d(5) - T_d(6)) - \frac{\rho_w V_d c^*_w}{200} (\Delta T_{d,5}),
\]
\[
H_{\text{av},6} = h_{d,\text{air}} A_{d,\text{air}} (6)(T_d(6) - T_{RM}) + h_d A_d (5)(T_d(6) - T_d(5))
- \frac{\rho_w V_d c^*_w}{200} \Delta T_{d,6}.
\]

The tank surface area exposed to air ($A_{d,\text{air}}(i)$) in tank $i$ and the area of the
common wall ($A_d(i)$) between tank $i$ and tank $i+1$ may vary from tank to tank.
The temperature $T_d(i)$ represents the average temperature in tank $i$ over the
period. Thus there is a system of six equations in two unknowns $h_d$ and $h_{d,\text{air}}$.
As the system is over determined the best solution is sought in the least squares
sense.

The parameter values during the idle phase of the experiment are listed in
table 7.4. The solutions for the heat transfer coefficients will of course be approx-
imate, so care is taken to err on the side of overestimating them. For this reason,
the water density adopted is for water at 65 °C, while quoted specific heat capac-
ity is for water at 95 °C. The system (7.3.6)–(7.3.11) can be written in matrix
form and solved for $h_d$ and $h_{d,\text{air}}$ using the least squares method. The solutions
give heat transfer coefficients of $h_d \approx 400 \text{ W m}^{-2} \text{ K}^{-1}$ and $h_{d,\text{air}} \approx 30 \text{ W m}^{-2} \text{ K}^{-1}$.
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<td>94.6</td>
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<td>0</td>
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<td>0.9</td>
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<tr>
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<td>810</td>
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<tr>
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<td>0.2458</td>
<td>0.2458</td>
<td>0.2458</td>
<td>0.2458</td>
<td>0.2999</td>
</tr>
</tbody>
</table>

**Table 7.4:** Parameter values during idle phase of experiment. Quoted water density is for water at 65 °C, while quoted specific heat capacity is for water at 95 °C.

The thermal resistance between two tanks $r_d$ is the reciprocal of the thermal conductivity. We can write this resistance $r_d$ as $r_d = r_w + r_{ss} + r_w = 2r_w + r_{ss}$, where $r_w$ is the thermal resistance of the water layer near the tank wall and $r_{ss}$ is the resistance of the stainless steel wall. The resistance of the stainless steel wall can be calculated from the ratio of its thickness, 0.0015 m, to its thermal conductivity 16.2 W m⁻¹ K⁻¹. Thus $r_{ss} = 9.26 \times 10^{-5} \text{m}^2 \text{K W}^{-1}$. The resistance of the water boundary layer is

$$ r_w = \frac{1}{2} (r_d - r_{ss}) = 0.0012037 \text{m}^2 \text{K W}^{-1}. \quad (7.3.12) $$

This gives a heat transfer coefficient for the water boundary layer of $h_w \approx 830 \text{W m}^{-2} \text{K}^{-1}$. The thermal conductivity of water at 65 °C is 0.659 W m⁻¹ K⁻¹ and so the length scale of the water boundary is approximately 0.0008 m.

For the heat transfer coefficient $h_{d,air}$, the thermal resistances of the water boundary layer and the stainless steel are small relative to the thermal resistance of the air boundary layer near the tank surface. Thus attributing all the thermal resistance to the air boundary we can estimate the length scale of this boundary as the ratio of the thermal conductivity of still air at room temperature 0.024 W m⁻¹ K⁻¹, to the heat transfer coefficient $h_{d,air} \approx 30 \text{W m}^{-2} \text{K}^{-1}$, to get a length scale of the air boundary of approximately 0.0008 m. Note that assuming that the thickness of the boundary layer for PG is the same as that estimated for air and water here, then the heat transfer coefficient for PG can be estimated. The thermal conductivity of PG at 95 °C is 0.1978 W m⁻¹ K⁻¹. Thus the heat
transfer coefficient for PG would be $247.25 \text{ W m}^{-2}\text{K}^{-1}$. The thermal losses from PG should be less than that for DI at the same temperature.

### 7.3.1.4 Experiment drawbacks

It is not possible to fit and validate energy transport models just using the experiment described above due to the limited amount of data collected. The main drawbacks were:

1. The main issue is that there was no measurement of fluid temperature within stacks or of the stacks themselves. Without this, it is impossible to estimate the energy losses occurring within the stacks. It is also impossible to estimate any energy losses which may be occurring from the system plumbing and shower-heads.

2. Lens front curves were only in place in the top four trays. It seems likely that if all front curves were in place, the contact area between the fluid and the stack would be increased, which may lead to increased energy losses in the stack.

3. There are some issues with heater control which may lead to dosing temperatures outside required ranges. PID controller behaviour responds to system disturbances including filling/emptying of stacks, back-flushing, and shutting on and off of dosing. Not all of these disturbances are included in the heat transport models, so exact controller behaviour cannot be replicated. Ensuring outlet temperature remains within the required tolerance of the set point may require improved PID control.

In order to address the first point, an experiment was conducted to estimate the heat losses a single stack. This experiment is described in the next section.

### 7.3.2 Single stack experiment with DI water

One of the simplest ways to estimate the energy loss in a stack at steady state is to measure the steady state temperature difference between fluid entering the stack and fluid exiting the stack. This will not reveal whether the main losses are from the stack surfaces, or the fluid surfaces within the stack, but will give the total energy lost by the fluid (by whatever mechanism) in transit through the
stack. With this in mind an experiment was set up where DI dosing was applied to a single stack. The key details of the experiment were as follows:

- A stack of 24 trays, with all front curves in place, was placed in a dosing stage.

- The experiment had no cycle time and was run from start to finish in the same stage.

- DI was delivered from the tank, at a set point of 95°C, through the shower-head to the stack at a rate of $5 \text{ l min}^{-1}$ throughout experiment.

- The stack entered at room temperature so was heated from cold.

- Before beginning the experiment, sufficient time was allowed for the fluid dosed through the shower-head to reach a steady state temperature. This temperature was 89.5°C. This was taken to be the entry temperature at the top of stack.

- Once fluid started exiting the stack its temperature was recorded every minute. The initial exiting temperature was for the first 0.5 l of fluid that exited.

The primary objective was to estimate the heat lost by the fluid as it cascades down through the stack. Some secondary objectives were as follows:

- To establish the volume of fluid contained in the stack at steady state.

- To establish the volume of fluid remaining is a stack after dosing has stopped.

- To establish the time taken for the fluid temperature to reach a steady state after dosing to the cold stack begins. This should reveal whether the load of heating a cold stack is fully borne by the first heater in the hydration system.
7.3.2.1 Experimental results

The measured temperature of the exiting fluid, along with the entry temperature at the top of the stack, is plotted in figure 7.10a. The temperature drop from the top to bottom of the stack is shown in figure 7.10b. After the shower-head was turned on above the stack it took 48 s for the fluid to exit the bottom of the stack. This indicated that the steady state volume in the stack is 4 l (for a 51 min$^{-1}$ dosing rate). This suggests that for a 30 tray stack, assuming a linear relationship, it would take 60 s for fluid to exit and it would contain 5 l at steady state, for the same dosing rate. After dosing was stopped it took 24 s for fluid to stop flowing out the bottom of the stack. This suggests that the volume of fluid retained in the stack following dosing is 2 l. For a stack of 30 trays this would be 2.5 l. Interestingly, tests show that each front curve can hold 0.4 ml of liquid. Thus the 1920 lenses in a 30 tray stack can retain 0.768 l. It is unclear where the remaining $\approx 1.7$ l of liquid is retained within the stack.

![Diagram](image.png)

**Figure 7.10:** (a) Steady temperature of fluid entering at top of stack and fluid exiting stack during single stack energy loss experiment. (b) Temperature drop $\Delta T$ from top of stack to bottom of stack during experiment. Note the steady state temperature drop marked on the figure is 3.2°C.

Once fluid starts exiting the stack, the temperature of the fluid is recorded every minute. The first 0.5 l of fluid collected measured 50°C. The exiting temperature is observed to quickly increase above 80°C around 2–3 minutes after dosing begins and reaches steady state within 4–5 minutes. The steady state exiting temperature is approximately 86.3°C, giving a steady state temperature drop of 3.2°C for the 24 trays. For a stack of 30 trays temperature loss would be around 4°C. It is notable that significant losses in temperature occur before the
7.3 Mini-stack rig experiments

fluid even enters the stack. There is a drop of temperature in the region of 5°C between the heater outlet and the fluid exiting the shower-head. This is greater than the total steady state drop in the stack. It is important that this loss is reduced as much as possible in the production line model. This should be easy to minimise as the piping and shower-head on the mini-stack rig is uninsulated. Also for the single stack experiment the system was not enclosed and open to room temperature in the Vistakon factory. The production line system will be an enclosed unit with a much higher ambient temperature. The stack entry temperature of 89.5°C will vary with heater outlet temperature due to set point errors arising from PID control. However, as the exact stack entry temperature was not measured in this experiment, the value of 89.5°C will be used. The heater outlet temperature and power output of the heater were also logged during the experiment. The steady state heater power output was approximately 15% or 2.7 kW. For DI with a flow rate of 5 l min$^{-1}$ this is consistent with a temperature loss of approximately 8°C between fluid exiting and entering the heater. This ties in with the measured losses of about 5°C between heater and stack and 3°C in stack before fluid re-enters tank.

7.3.2.2 Experiment analysis

From the results it is simple to estimate the energy lost per second in the stack. This equates to the power that the heater must supply to recover this energy. The flow rate into and out of the stack $Q$, is 51 l min$^{-1}$. The temperature drop $\Delta T$ is 4°C. The water density and specific heat capacity are taken to be approximately 980 kg m$^{-3}$ and 4200 J kg$^{-1}$ K$^{-1}$. The energy lost per second ($\Delta P$) is given by:

$$\Delta P = Q \rho_w c_w \Delta T.$$  (7.3.13)

Thus the steady state energy loss per second in a 30 tray stack is approximately 1.4 kW. As was mentioned above the available data does not allow the nature of the losses to be determined. One option is to assume that at steady state most of the energy lost in the stack is from the stack surface. This allows an effective heat transfer coefficient to be determined which specifies the energy lost per second through a unit area of the stack surface when a 1 K temperature difference is maintained between the stack and the air. This is based on the assumption that the stack temperature is approximately the same as the fluid temperature. The
7. HEAT TRANSPORT IN THE CONTACT LENS HYDRATION PROCESS

thermal conductivity of the stack material (Ultem HU1004) is 0.19 W m\(^{-1}\) K\(^{-1}\) so it is quite a good insulator. However, this value is still an order of magnitude greater than that of still air, so the assumption that the stack temperature is close to that of the fluid may not be unreasonable. Assuming all energy lost is from the stack surfaces the heat transfer coefficient can be found using

\[ h_{c,\text{air}} = \frac{\Delta P}{A_{c,\text{air}}(T_e - T_{RM})}. \] (7.3.14)

The stack temperature is assumed to be approximately that of the fluid so that \(T_e \approx 86^\circ\text{C}\). Room temperature \(T_{RM}\) is 23\(^\circ\text{C}\). The stack dimensions are 0.26 m \(\times\) 0.279 m \(\times\) 0.45 m. This means the total stack surface area (excluding top and bottom and internal tray surfaces) is \(A_{c,\text{air}} = 0.4851 \text{ m}^2\). Thus the heat transfer coefficient is estimated as \(h_{c,\text{air}} = 45.8 \text{ W m}^{-2}\text{K}^{-1}\). This value is somewhat higher than the heat transfer coefficient of 30 W m\(^{-2}\) K\(^{-1}\) found for the tank to air losses. However, as the stack to air heat transfer coefficient also incorporates other possible losses in the stack, including direct fluid to air losses and losses through evaporation, the value does not seem unreasonable. It is difficult to draw any other conclusions except to mention that, given the non-ideal conditions of the experiment, stack energy losses in practice should not exceed those observed here. Thus, the heat transfer coefficient calculated here should give a reasonable estimate of the worst case energy losses from a stack.

Steady state losses in stack for PG dosing  Unfortunately, it was not possible to obtain data for losses in a single stack during PG dosing. The following comments are made:

- If we assume all losses are from the stack surface, then using PG should not change the heat transfer coefficient.

- The thermal conductivity of PG is about one third that of water for still fluid. Based on this one would expect DI to heat the stack quicker and maintain a higher stack temperature than PG. This would lead to lower losses for PG than DI.

- The specific heat capacity of water is higher than that of PG which is approximately 2900 J kg\(^{-1}\) K\(^{-1}\). For the same energy loss the temperature
drop in PG temperature will be bigger. For example a 4°C drop for DI would be approximately a 5.8°C for PG for the same energy loss.

- PG is less volatile than water (its vapour pressure is an order of magnitude lower than water) but has a slightly higher latent heat of vaporization. Thus PG evaporates a lot less than water but when it does the remaining fluid loses slightly more energy. Thus any such losses should be less for PG.

Based on the above discussion, it seems reasonable to assume that energy losses in a stack with PG will not be more than that for DI. However there is not sufficient evidence to determine if energy losses are significantly less. Thus heat transfer coefficient fitted here for DI, will also be applied for modelling of energy losses in PG stacks.

**Energy needed to heat stack** When a stack at room temperature enters the hydration system significant energy is lost from the hydrating fluid initially in the heating of the stack. The energy requirement to heat a stack from room temperature depends on the specific heat capacity of the tray material $c_e$. The heat capacity of Ultem HU1004 was requested from manufacturers Sabic Innovative Plastics. Data from Sabic is shown in figure 7.11. The heat capacity of Ultem depends strongly on temperature. Two curves plotting specific heat capacity against temperature are shown in the figure. The lower curve was measured while heating the Ultem from just above 0°C to about 400°C. The upper curve was measured while cooling the material through this temperature range. To ensure the energy demand is not underestimated the value of heat capacity for Ultem is set to 1100 J kg$^{-1}$ K$^{-1}$ which roughly corresponds to the value of the specific heat capacity for Ultem at 95°C given by the upper curve. As the specific heat capacity is lower at lower temperatures, the actual energy required during stack heating should be significantly less. The energy required to heat the Ultem stack, of mass $m_e$, to an equilibrium temperature $T_{eq}$ is simply given by

$$m_e c_e(T_{eq} - T_{RM}). \quad (7.3.15)$$

Each tray in a stack has a mass of 0.5 kg. Thus the 24 tray and 30 tray stacks have masses of 12 kg and 15 kg respectively. If we assume that the stacks in the experiment reach an average temperature which is close to the steady state exiting
fluid temperature, say 86°C, then the total energy required is approximately 832 kJ. Averaging this over the cycle time would require an average power output of approximately 1.85 kW. Scaling this up to a 30 tray stack the total energy and average power requirements would be 1040 kJ and 2.3 kW. If we assume that the stacks on the production line actually reach the set point temperature of the fluid, than the total energy and average power requirements would be 1188 kJ and 2.64 kW. Of course these figures do not include the steady state losses outlined above. The requirement to maintain set point temperature means that the instantaneous power requirement will be much higher initially when the first cold fluid exits the stack into the tank. Maintaining a volume of hot fluid in the tank will insulate the heater somewhat from having to recover the full fluid heat loss instantaneously.

Returning to the experimental data, the temperature drop data in figure 7.10b can be used to estimate the total energy demand, average power requirement over a cycle and average power requirement in each minute to recover energy loss in the stack. The data can also be used to get a rough estimate of the energy which goes in to heating the stack by deducting the steady state loss. If this is similar to the total calculated energy requirement for stack heating, we can conclude that the
7.3 Mini-stack rig experiments

Figure 7.12: Temperature drop data extrapolated for a 30 tray stack. Data is fitted by the function $\Delta T(t) = 4 + 45.35e^{-0.022493t}$, where $t = 0$ is the time when first fluid begins to exit stack (48 s after dosing starts).

steady state stack temperature is close to that of the fluid. Calculations here will be done on the basis of a 30 tray stack, so where required temperature drops etc. are scaled linearly with the number of trays. If the initial stack outlet temperature is near room temperature, approximating the temperature drop as increasing linearly with the number of trays will not work well. However, as the initial exiting temperature is still well above the room temperature, and the increase in the number of trays is relatively small, the linear scaling will be adopted here. In order to estimate the total energy lost in a stack, initially at room temperature, over a cycle time, the energy loss per unit time given by equation (7.3.13) is integrated over the cycle time. As the temperature drop data is only recorded every 60 s, the integral can be estimated either using a quadrature rule, such as the trapezoidal rule, or by fitting the data with a continuous function. Here the data is fitted by an exponentially decaying function of the form $a + be^{-ct}$, where $a$, $b$ and $c$ are fitting constants. The best fit to the data with $a = 4.00$, $b = 45.35$ and $c = 0.022493$. The constant $a$ represents the steady state temperature drop. The start time $t = 0$, is the time when fluid initially starts to exit the stack. The
7. HEAT TRANSPORT IN THE CONTACT LENS HYDRATION PROCESS

Total energy lost between \( t = 0 \) and an arbitrary time \( t = t^* \) is given by:

\[
\Delta E_{\text{total}}(t^*) = \int_0^{t^*} Q \rho_w c_w \Delta T(t) \, dt \\
= \int_0^{t^*} Q \rho_w c_w (a + be^{-ct}) \, dt \\
= \frac{Q \rho_w c_w}{c} \left( b(1 - e^{-ct}) + act^* \right). \tag{7.3.16}
\]

Setting \( a = 0 \) removes the steady state loses and gives an estimate of the heat energy used to heat the stack to steady state. Of course the steady state loses may be less while the stack is heating from cold so heat energy delivered in heating the stack may be underestimated. The plots of total energy loss during experiment with \( a = 0 \) and \( a = 4 \) are shown in figure 7.13. The total energy delivered to heating the stack is just over 706 kJ. This is a bit less than the total 1040 kJ calculated earlier for heating a stack to steady state. However, given that the average specific heat capacity of Ultem during heating may be more like 900 J kg\(^{-1}\) K\(^{-1}\) than 1100 J kg\(^{-1}\) K\(^{-1}\), and the other losses during the initial phase are probably less than that at steady state, it seems likely that the average stack temperature is close to that of the hydration fluid. Thus the heater in the first stage does (at least in the case of DI) have to supply enough energy to heat the cold stack to set point temperature within one cycle and should be sized accordingly. Based on this experiment the average power requirement over the first cycle to heat a stack of 30 trays and recover steady state losses in the stack is approximately 3.2 kW. Note that losses from the tank surfaces, system plumbing and shower-heads have to be added to this figure.

The timescale on which a stack is heated is given by \( \frac{1}{c} \approx 45 \text{ s} \) and stack reaches steady state temperature about 2 min after water exits stack. If the heater inlet came directly from the stack outlet than a large heater would be required to maintain set point. For example, a 9 kW heater can make up a temperature difference of about 27 °C for water with a flow rate of 51 min\(^{-1}\). For PG at the same flow rate a temperature difference of about 36 °C could be recovered. For the production line, with two stacks the flow rate through the heater would be doubled and so the same heater could only make up a temperature difference half as big. Fortunately, the hydration fluid is returned to the tank before going into the heater, and so by managing the tank temperature and volume effectively it
should be possible to insulate the heater in stage 1 from this large load over the first 2–3 minutes of the dosing cycle. Some consideration will be given later in the chapter, to how such an approach can be used to ensure the heater in stage 1 does not have to be excessively large, just to meet the initial spike in energy demand.

7.3.3 Fitting model to mini-stack rig DI experiments

The data from the mini-stack rig experiments, described above, has allowed certain fitting parameters to be estimated. In this section the output of the cycle averaged heat transport model and the compartment model for energy transport during dosing will be compared with the data obtained by running all stages in the mini-stack rig with DI.

7.3.3.1 Cycle averaged model

The cycle averaged model in section 7.2.4 gives an estimate of the average heater demand per cycle. The predicted power demand of the model can be compared with the average power delivered per cycle from the experimental data. It can also be used to identify where the power demands in each stage are originating. The model gives an estimate of the average power demand during dosing and
so does not account for changes in the flow paths during backflush and move time. Thus the average demand will be overestimated. It is quite easy to adjust the model to account for changing demand in backflush and move time, but the dosing time is the most important, as it sees the highest demand.

The model output is compared to the average power output from experiment over the cycle time and during the actual dosing time (345 s) in figure 7.14a. The heat transfer coefficient from the stack surface to the air is taken from the single stack experiment. This is likely too high as all front curves were not in place for the full system experiment. The results show that the model does indeed overestimate the average power demand for each stage, but nonetheless provides a reasonable estimate considering the simplicity of the model. The breakdown of the power requirements in each stage are shown in figure 7.14b. The biggest demands are the heating of DI in stages 5 and 6. In fact the total demand in heater 6 is just above the heater wattage of 18 kW. In the experiment the heater ran at an average of about 15.5 kW and was just below set point during dosing. The fact that the set point was attained might suggest that the actual entry temperature of DI was above the 25°C assumed in the model. Also the load of heating incoming DI was not present when dosing was stopping during experiments, which has not been accounted for in the model. Similarly the large demand to heat incoming DI at 40°C in stage 5 is only present for 345 s of the cycle in the experiment, whereas the model accounts for this load for the full cycle time. The losses of heat energy from the tank surfaces to air are relatively small but still account for an average of up to 0.6 kW power loss per stage. It should be relatively easy to reduce this loss by insulating tanks on the production line system. The tank to tank transfer between adjacent ‘PG’ and DI tanks is about 0.5 kW. As discussed earlier there is a significant load in the first stage of up to 2.64 kW to heat cold stack to set temperature. The stack also transfers heat to the fluid in stage 4 as it cools, reducing the power requirement there.

7.3.3.2 Compartment model

The full compartment model in section 7.2.2 describes energy transport between compartments during the dosing cycle. The changes in the energy transfers during the backflush and move time are not accounted for. This can be done by specifying different energy transport equations for the three periods of the dosing cycle, and solving them in sequence for their respective times. Here, to avoid the extra
complexity, the dosing time equations are solved for full cycle time. The loads during backflush and move time are less than or equal to those during dosing so the load prediction should not be significantly different. The model will not be able to exactly replicate PI controller behaviour from experiments as it does not include the same system disturbances. However the behaviour should be qualitatively similar. Heater operation is simulated using the algorithm described in section 7.3.1.2 with some minor adjustments to ensure the stability of the simulations.

The key adjustment made is to incorporate a time delay in the implementation, by the heater, of the control signal $CO(t)$ at time $t$. Suppose the wattage associated with $CO(t)$ for a particular heater is $W_{CO}(t)$. Then the heater wattage delivered, $W_{heater}(t)$, is determined by

$$\frac{dW_{heater}}{dt} = \frac{1}{t_{\text{delay}}} \left( W_{CO} - W_{heater} \right), \quad (7.3.17)$$

where $t_{\text{delay}}$ is a delay time over which the heater responds to the control signal.

The operation of heaters in the simulations is simply a response to the simulated outlet temperatures and vice-versa. Given the modelling simplifications, it is not expected that the PI-control data from experiments can be replicated. The aim is to replicate the general range of wattage demand seen in experiments in each stage.

The heater wattage and outlet temperatures from heaters 1 and 4, over the 219
first four cycles from experiment, are compared with the simulated results in figure 7.15. The simulations started with all tanks and stacks at room temperature and simulated a number of dosing cycles. The model was not adjusted to shut off dosing while tanks were warming up to temperature. Thus the phase of the simulations has been a shifted to line up with the experimental results. Despite not accounting for system changes during and backflush and move time, the model shows very good agreement with the data for both heater wattage (figure 7.15a) and outlet temperature (figure 7.15b) for heater 1. The results for heater 1 show the best agreement between model output and collected data. The worst agreement is shown by heater 4 in figures 7.15c and 7.15d. It can be seen that the temperature variations are much larger in the simulations than in the data. The reason for this may be down to a reduced transfer of energy from the hot stack in experiments relative to simulations. In the experiments no dosing takes place to stage 3 during backflush or move time (105 s). The stack temperature may drop significantly during this period and so has significantly less energy to transfer to the cooler fluid in stage 4. This is not accounted for in the model.

The model can also produce other outputs to understand the system operation. The simulated tank temperature and heater outlet temperatures in stage 1 are shown in figure 7.16a. Based on the tank temperature, we can calculate the ideal heater operation to reach outlet temperature at each time and compare this to the PI signal and the actual heater operation as determined by the time delay $t_{\text{delay}}$. The heater demand is compared with the PI signal and the wattage delivered in figure 7.16b. Also included is the cycle averaged estimate of power requirement. The time delay chosen is small, so the PI signal and delivered wattage almost coincide. It can be seen that the delivered wattage lags behind the wattage demand, resulting in a significant dip in tank and outlet temperatures. The controller can then be seen to adjust for the increased load and overshoot the set point later in the dosing cycle.

The temperatures of all compartments, once the system has reached steady cyclic operation, can also be plotted from the simulations as shown in figure 7.17. The heater outlet temperature and tank temperature are shown for all the five stages and for the preheat tank. The stack and fluid in stack compartment temperatures are shown for the five stages. The time on the horizontal axis corresponds the time since a particular stack enters the system. For example, the stack is in the third stage from 900 s to 1350 s and so the temperatures of
Figure 7.15: Comparison between compartment model simulations and experimental data from mini-stack rig DI experiments for (a) wattage delivered in heater 1, (b) outlet temperature in heater 1, (c) wattage delivered in heater 4, (d) outlet temperature in heater 4.

compartments in stage 3 are shown on this range. The preheat compartment temperatures during a cycle are shown on the range 2250 s to 2700 s. The stack in stage 5 is dosed with DI at 40 °C leading to the lower stack and fluid in stack temperatures seen in the plot. The energy density is assumed uniform within a stack, so no spatial temperature gradients are modelled. The temperature of the fluid in stack compartment should approach that of the fluid exiting the stack in experiments.

7.3.4 Mini-stack experiments with PG and DI

Only one experiment is available in which the first three stages of the mini-stack rig run PG and the final two stages run DI as intended. There is no data on
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Figure 7.16: (a) Modelled tank and outlet temperature in heater 1. (b) Comparison between ideal heater operation and heater operation as implemented by PI controller simulation. Result from cycle averaged model also included.

The temperature trace of a stack as it goes through the system is shown in figure 7.18a. The start of dosing can be identified by the rapid jump in the temperature at the top centre position at around 200 s on the plot. The temperature at the bottom centre begins to rise quickly at about 230 s. This indicates that

<table>
<thead>
<tr>
<th>Stage</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flow rate (L/min)</td>
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<td>5.0</td>
<td>1.0</td>
<td>5.0</td>
<td>1.0</td>
<td>5.0</td>
</tr>
<tr>
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<td>PG</td>
<td>DI</td>
<td>DI</td>
<td>PG</td>
</tr>
<tr>
<td>Temp set point (°C)</td>
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<td>88</td>
<td>88</td>
<td>65</td>
<td>65</td>
<td>88</td>
</tr>
<tr>
<td>Cycle time (s)</td>
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<td>450</td>
<td>450</td>
<td>450</td>
<td>450</td>
<td>450</td>
</tr>
<tr>
<td>Backflush time (s)</td>
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<td>60</td>
<td>60</td>
<td>60</td>
<td>60</td>
<td>60</td>
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<tr>
<td>Move time (s)</td>
<td>30</td>
<td>30</td>
<td>30</td>
<td>30</td>
<td>30</td>
<td>30</td>
</tr>
</tbody>
</table>

Table 7.5: System parameters for mini-stack PG-DI experiments.

7.3.4.1 Experimental observations

The temperature trace of a stack as it goes through the system is shown in figure 7.18a. The start of dosing can be identified by the rapid jump in the temperature at the top centre position at around 200 s on the plot. The temperature at the bottom centre begins to rise quickly at about 230 s. This indicates that
fluid takes about 30 s to work its way down through the stack, compared to the
60 s inferred from the DI experiment. It is unclear which this is related to the
differing properties of the liquid (for example the viscosity of PG is an order of
magnitude greater than that for water), or perhaps that the front curves were
not all in place for this experiment. If the former is the case, the steady state
volume of PG in the stack may be 2.5 l rather than 5 l. The top centre tempera-
ture increases rapidly, stabilises, and then briefly dips, before recovering and over
shooting the set point. The dip is likely in response to the initial cold PG exit-
ing the stack causing a drop in tank temperature. The overshoot to 92 °C (4 °C
above set point) is likely a PID control issue. Interestingly, if there is significant
temperature loss between the heater outlet and the top of the stack, the actual
overshoot may be more than this. In the second stage, the top centre temperature
stays close to its set point of 88 °C. In the third stage, the temperature at the
top centre position varies between 84 °C and 86 °C. The lower temperature here
is probably due to the low flow rate of 11 min\(^{-1}\) into stage 3. From the available
data, it not possible to determine with any certainty whether the reduced tem-
perature is due to increased losses in the piping between the heater outlet and
the stack or the lower flow rate leading to a lower equilibrium stack temperature and hence reduced fluid temperature.

The temperatures at the bottom corner position are lower than the top centre position but generally track the changes in temperature in the top position with a lag time of about 30 s, corresponding to the time taken for the PG to transit through the stack. The temperature difference between top and bottom is quite variable. After the initial stack heating, the temperature difference generally reduces over the first three stages. The temperature difference reduces from 4°C to 8°C in stage 1 to 2°C to 4°C in stage 2 to 1°C to 3°C in stage 3. These results seem to indicate that PG takes a little longer than DI to reach steady state temperatures in the stack. This is not surprising as PG is less efficient at transferring heat energy to the stack. Either of the temperature drop ranges representative of stages 2 and 3, support the idea that the energy loss in a stack at steady state using PG is less than that for DI. The lower temperature drop in stage 3 is somewhat counter-intuitive. One might expect a much higher temperature difference in this stack due to the lower flow rate. A separate experiment was conducted where a cold stack starting at room temperature was dosed with PG at 11 min\(^{-1}\). The temperature traces from the top and bottom are shown until the temperature difference reaches steady state in figure 7.18b. Here a temperature drop of over 15°C is evident. The discrepancy between these two observations can be explained by assuming that, in the case of the full dosing cycle, the hot stack is providing enough energy to the fluid to limit the energy loss from the fluid as it transits through the stack. Over time, as the stack cools, one would expect the behaviour to transition to that in figure 7.18b but over one dosing cycle there seems to be sufficient heat energy in the stack to maintain a small temperature drop.

In stage 4, the first DI stage, both temperature traces exceed the set point. In fact the bottom temperature trace sometimes exceeds the top one. In this case DI is actually cooling down the hot stack that has exited the PG stages and so is picking up energy from the stack. In the final stage the temperature drops off below the set point at both the top and bottom positions. This again suggests that the lower flow rate results in a lower equilibrium temperature in the stack (assuming there are no control issues). The temperature traces in the final stack are still decreasing when dosing stops.
7.3.4.2 Experiment drawbacks

Running the mini-stack rig with PG and DI should give the best data to fit the energy transport models. However given the limited data collected it is not possible to fit the individual energy transfers. To do this the experiments running DI will be used and the ability of the fitted coefficients to reproduce the temperature traces observed in the PG and DI experiment will be considered.

7.3.5 Fitting model to mini-stack rig PG and DI experiments

In this section the compartment model will be used to simulate the mini-stack rig PG and DI experiments. The available data, for comparison with the model output, is the temperature traces from the top and bottom of stacks presented in the previous section. Given the somewhat limited information on this experiment, a certain amount of guess work will have to be relied on to set up the model parameters for simulation. It is not known how long the system had been running before the data was collected, so it is difficult to know if the temperature trace is really reflective of steady state behaviour. Also the system is enclosed for this experiment, but a room temperature of 23 °C will still be assumed. The key difference to the DI experiments is of course that the first three stages now run...
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PG. Thus parameters associated with the hydration fluid in these stages such as density, thermal conductivity and specific heat capacity are adjusted to those for PG. The energy loss from a stack for PG relative to water is more difficult to account for. With the exception of the stacks at the end, the stacks in this experiment have only two faces exposed to air (the other two are in contact with the neighbouring stack). Thus the area for loss to air may be effectively halved. Any stack to stack transfer is neglected. The heat loss does not necessarily scale with stack surface area though, as evaporative losses may make up a significant part of the fitted heat transfer coefficient. In this instance, the stack surface areas will be adjusted to take account of the neighbouring stacks and the heat transfer coefficients will be adjusted as necessary to better fit the temperature traces. Given the uncertainty over the experimental conditions and source of the stack losses, when the model is applied to the production line system, the total loss observed in the single stack experiment with DI will be incorporated. This conservative approach will minimise the risk of under-sizing the heaters required.

![Figure 7.19](image.png)

**Figure 7.19:** (a) Comparison between temperature profile produced by model simulation for fluid in stack and experimental temperature traces. (b) Temperature profiles produced by model simulations of the PG and DI mini-stack rig experiments.

The simulated temperatures of fluid in stacks during hydration are compared with the top and bottom temperature traces from experiment in figure 7.19a. In general the agreement is quite good except during the heating phase in the first stage. This is not surprising as the model does not incorporate the filling of the first stack. Thus the volume of fluid in the first stack needs to be assigned
an initial temperature at the start of each cycle. Here the fluid is set to room temperature. This will overestimate the heater demand initially and lead to a longer heating up phase as can be seen in the figure. The absence of filling and emptying has less influence on the other stacks as they will empty less and should largely maintain temperature during the move time. The limitations of the model due to not modelling fluid volume changes in stacks and tanks will be discussed when modelling energy transport on the production line system. In particular the initial filling phase in stage 1 will be considered in more detail. The model also produces the wattage delivered by the simulated PI controlled heaters. This output is not plotted here as there is no data with which to compare.

7.4 Heater size estimates for production line hydration system

In the previous sections it has been shown that cycle averaged and time dependent compartment models of energy transport in the mini-stack rig hydration system, can be used to provide estimates of the energy demand on heaters in each stage to maintain the required processing temperatures. Where simplifying assumptions are made about the process, care is taken to ensure that these assumptions tend to overestimate the demand on heaters. Thus the cycle averaged model should tend to overestimate the average steady state power requirement in each stage over a dosing cycle. The time dependent compartment model produces an estimate of the wattage delivered by the PI controlled heaters during the dosing cycle. This may differ from the actual demand, so the instantaneous demand is also calculated. Note the demand on the system depends on the previous actions of the heaters. If the control of the heaters is sub-optimal (depending on the PI controller tuning), this can lead to higher demand than necessary if optimal control could be achieved. For this reason the PI controller is simulated using the parameters from controllers in the mini-stack rig. The heaters will be sized sufficiently large to meet either the highest instantaneous demand observed in a stage over a dosing cycle or the highest instantaneous power delivered (which ever is larger). It may be possible to reduce the peak demand by improving the control algorithm, but this will not be assumed here. Thus we will proceed as follows:
1. Consider the condition that the heaters must deliver a cold start-up time of less than 30 minutes to establish a lower bound for heater size in each stage.

2. Rewrite the cycle averaged model for the production line system, adapting energy transfer terms where possible/necessary. Use the model to provide initial estimates of the average power requirements in each stage. Also consider which are the main components of the power requirement in each stage.

3. Rewrite the full compartment model for the production line system again adapting energy transfer terms where possible/necessary. Use the model to provide estimates of peak power requirements in each stage. Compare to that of the cycle averaged model. The model can also be used to investigate optimal operation of heaters. One other question is whether recirculation of hydration fluid through heaters to maintain tank temperature is beneficial or whether it is better to use all of a heater’s capacity to heat fluid going to the shower-heads?

4. Investigate whether any of the assumptions made in the models may lead to an underestimation of the peak power requirements in the system. In particular whether the filling and emptying of stacks and tanks has any major impact on power demand.

### 7.4.1 Cold start-up time

As outlined in section 6.4.2, the production line system has 9 tanks each of which has a capacity of about 301. Tank 7 is always empty and has no heater attached. Each of the other tanks has its own heater except tank 8 which has 2 heaters as it supplies both stages 7 and 8. Unlike in the mini-stack rig, the tanks are insulated on the sides, bottom and ends by 16 mm EPDM elastomeric sheet insulation. This reduces the heat loss from the tanks surfaces. The dimensions of a single tank (not to scale) are shown in figure 7.20. Note the configuration of tanks is different in the production line system. The PG tanks (1–5) are built in one piece with common walls and sit under their respective stacks. The preheat tank is a separate tank and sits under the stack in stage 6. A catch pan over the preheat tank delivers fluid from stack 6 directly into tank 5. The DI tanks (7–9) are also
7.4 Heater size estimates for production line hydration system

built in one piece with common walls, but tank 7 runs empty. DI from the stack in stage 7 runs into it, but exits directly to be collected in a DI effluent tank. Thus the heat transfer between adjacent PG and DI tanks will not be an issue on the production line system.

Figure 7.20: Dimensions of one tank in production line system. (Dimensions are in metres).

For the purposes of calculating the energy needed for a cold start-up, a single tank is considered and interactions between tanks are neglected. The energy needed to heat tank full with 30 l of PG from room temperature (23°C) to a set point of 96°C can be quickly calculated from the total mass and specific heat capacity of PG. In reality PG can be delivered from factory sources at 60°C so if this is done the start up times calculated here will be approximately halved. Noting the density of PG at room temperature is about 1032 kg m\(^{-3}\), the total mass of PG is approximately 31 kg. The specific heat capacity is taken to be 2900 J kg\(^{-1}\) K\(^{-1}\) and the increase in temperature is 73°C. Thus the required energy is

$$m_p c_p \Delta T_p = 6562.7 \text{ kJ.}$$

The energy required to heat the stainless steel tank can also be easily estimated. The surface area of the tank is approximately 0.5 m\(^2\). Thus the volume of stainless steel in the 2 mm sheets making up the tanks is approximately 0.001 m\(^3\). The density of stainless steel is approximately 7800 kg m\(^{-3}\). Its specific heat capacity is 510 J kg\(^{-1}\) K\(^{-1}\) and the temperature change again is 73°C. Thus the required energy is

$$V_{ss} \rho_{ss} c_{ss} \Delta T_{ss} = 290.4 \text{ kJ.}$$
Table 7.6: Estimates of cold start-up times for PG and DI tanks on production line based on heater wattage choice

<table>
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<th>Heater size (kW)</th>
<th>3</th>
<th>6</th>
<th>9</th>
<th>12</th>
<th>15</th>
<th>18</th>
</tr>
</thead>
<tbody>
<tr>
<td>Start-up time PG (min)</td>
<td>42.3</td>
<td>21.2</td>
<td>14.1</td>
<td>10.6</td>
<td>8.5</td>
<td>7.1</td>
</tr>
<tr>
<td>Start-up time DI (min)</td>
<td>25.6</td>
<td>12.8</td>
<td>8.5</td>
<td>6.4</td>
<td>5.1</td>
<td>4.3</td>
</tr>
</tbody>
</table>

Note the energy required to change the stainless steel temperature is much less than that for the PG and so has been neglected in the compartment models earlier. Thus the total energy required neglecting losses through tank surfaces is 6853.1 kJ. The start-up times (in seconds) can be estimated by dividing this figure by the quoted heater wattage times its efficiency (90%). Similarly the energy required to heat DI water and its stainless steel tank from room temperature to a set point of 55°C is approximately 4141 kJ. This start up time is usually not an issue as DI can be sourced from factory sources at 60°C. The estimated start up times in minutes for different heater sizes for PG and DI tanks are given in table 7.6. It is clear that only the 3 kW heater on PG tanks fails to meet the required cold start up time. Thus a lower bound for the heater sizes on PG tanks is 6 kW.

It is useful at this stage to calculate the new heat transfer coefficient for the loss of heat through the tank walls to the surrounding air, allowing for the added thermal resistance of the insulation. The insulating material has a thermal conductivity of 0.245 W m⁻¹ K⁻¹. Thus it thermal resistance is given by \( r_{\text{insul}} = \frac{0.016}{0.245} = 0.0653 \text{ K m}^2 \text{ W}^{-1} \). The total thermal resistance of the tanks wall is given by \( r_{\text{PG}} + r_{\text{ss}} + r_{\text{insul}} + r_{\text{air}} = 0.1026 \text{ K m}^2 \text{ W}^{-1} \) where the values for the other thermal resistances have been substituted from those used on the mini-stack rig. Thus the heat transfer coefficient is approximately \( h_{d,\text{air}} = 10 \text{ W m}^{-2} \text{ K}^{-1} \). Taking the worst case during the start-up period of a temperature difference of 73°C between the PG in the tank and the surroundings the power loss would be less than 0.4 kW. Assuming the average loss is about half of this the start-up time for a 6 kW heater would only rise to about 22 min. Thus the 6 kW lower bound remains valid for PG tanks. There is no restriction on the choice of heater for the DI tanks due to start-up times.
7.4 Heater size estimates for production line hydration system

Figure 7.21: Flows between compartments on production line system during dosing cycle for PG stages (1–6). PG enters at the preheat tank in stage six and is heated to set point before entering the system at the top of the stacks in stage 6. Stacks move from left to right after each cycle. The stacks entering the first stage are at room temperature. The stacks exiting enter the DI dosing stages.

7.4.2 Cycle averaged model

The cycle averaged model needs to be adapted to account for the changes in the energy transfers which occur on the production line system. The production line system has 11 stages in total. There are 6 PG stages, 4 DI stages and 1 stage called the destack stage where the stacks are intermittently dosed with DI while the stack is being dismantled. The system is equipped with 9 heaters to meet energy demands in the 11 stages. The flow paths in the PG stages during dosing are shown in figure 7.21. The flow paths in the DI dosing stages are shown in figure 7.22. Note the stacks in stage 10 and the destack stage, both empty into tank 9 and so add up to the refresh flow in the system. Tank 8 supplies both the stacks in stage 8 and the stacks in stage 7. The stacks in stage 7 drain directly to DI effluent storage through tank 7 which runs empty and so is essentially a catch pan for the exiting DI.

The equations for the cycle averaged heater demand on the production line
are given by:

\[ H_{av,1} = \frac{\rho_c V e c^*}{t_w} (T_1 - T_{RM}) \]
\[ + (h_{e,air} A_{e,air} + h_{d,air} A_{d,air} + h_{a,air} A_{a,air})(T_1 - T_{RM}), \]  
(7.4.3)

\[ H_{av,2} = (h_{e,air} A_{e,air} + h_{d,air} A_{d,air} + h_{a,air} A_{a,air})(T_1 - T_{RM}), \]  
(7.4.4)

\[ H_{av,3} = (h_{e,air} A_{e,air} + h_{d,air} A_{d,air} + h_{a,air} A_{a,air})(T_1 - T_{RM}), \]  
(7.4.5)

\[ H_{av,4} = (h_{e,air} A_{e,air} + h_{d,air} A_{d,air} + h_{a,air} A_{a,air})(T_1 - T_{RM}), \]  
(7.4.6)

\[ H_{av,5} = (2h_{e,air} A_{e,air} + h_{d,air} A_{d,air} + 2h_{a,air} A_{a,air})(T_1 - T_{RM}), \]  
(7.4.7)

\[ H_{av,6} = (h_{d,air} A_{d,air} + Q_{1(6)} \rho_w c_w^*) (T_1 - T_3), \]  
(7.4.8)

\[ H_{av,7} = \frac{1}{2} (h_{e,air} A_{e,air} + h_{d,air} A_{d,air} + h_{a,air} A_{a,air})(T_2 - T_{RM}), \]  
(7.4.9)

\[ H_{av,8} = \frac{1}{2} (h_{e,air} A_{e,air} + h_{d,air} A_{d,air} + h_{a,air} A_{a,air})(T_2 - T_{RM}), \]  
(7.4.10)

\[ H_{av,9} = (h_{e,air} A_{e,air} + h_{d,air} A_{d,air} + h_{a,air} A_{a,air})(T_2 - T_{RM}) \]
\[ + Q_{1(11)} \rho_w c_w^* (T_2 - T_4) + Q_{1(11)} \rho_w c_w^* (T_2 - T_4) \]
\[ + 2(h_{e,air} A_{e,air} + h_{a,air} A_{a,air})(T_4 - T_{RM}) - \frac{\rho_c V e c^*}{t_w}(T_2 - T_4). \]  
(7.4.11)

As with the mini-stack rig model, \( T_1 \) and \( T_2 \) are the set point temperatures for PG and DI respectively. The temperature \( T_3 \) is the temperature of the PG entering the preheat tank. On the production line this will be 60°C instead of room temperature. The temperature \( T_4 \) is the temperature of the incoming DI
and will be taken as 55°C. Note the DI set point $T_2$ may be different to this, but if it isn’t, a number of the terms in the demand equation for heater 9 drop out. The volume flow rate $Q_1(i)$ now depends on stage number and represents the refresh or weiring flow out of stage $i$. For example the volume flow rate out of stage 9 is the sum of the volume flow rates entering stage 9 from stages 10 and 11 (destack stage). There is no heat transfer via conduction between adjacent PG and DI tanks as tank 7 is now empty. The two heaters on tank 8 are numbered according to the stage they supply. It is assumed that the heaters divide the load of recovering energy lost in stage 8. Any energy lost in stacks, or gained from a hot stack exiting the PG dosing stages in stage 7, does not have to be accounted for as DI exits the system directly from stack 7. The heat transfer from fluid in stack to air $h_{d,\text{air}}$ will be set to zero as with the mini-stack rig. The fitted value for $h_{e,\text{air}}$ will be used to incorporate these losses. Although not explicitly indicated, the heat transfer coefficient for losses from tank to air, $h_{d,\text{air}}$, and tank surface area for loss, $A_{d,\text{air}}$, will both vary depending on stage number. The area $A_{d,\text{air}}$ can be calculated from the tank dimensions. Tanks at the ends have a larger area exposed to air. The heat transfer coefficients $h_{d,\text{air}}$ can be calculated as the inverse of the total thermal resistance of the tank wall between the hydration fluid and the surrounding air. This will be slightly different for PG and DI. The values of the model parameters used to calculate the steady state loads on the system heaters are listed in table 7.7. Where appropriate some references to material data sheets are given. Note the mass of the two stacks, $m_e$ has been given, rather than the density and volume.

The resulting predictions of the average power requirement for each heater over a cycle are shown in figure 7.23a. Figure 7.23b gives the breakdown of the sources of the energy requirements for each heater. Heaters 7 and 8 have a very low power requirement of less than 1 kW, which is unsurprising as they split the load of recovering the losses in stage 8 between them. The power requirement on heater 9 is quite large at almost 4.5 kW. This is due to the fact that this tank must recover losses in stacks in stages 9, 10 and 11, as can be seen by the large stack to air component for heater 9 in figure 7.23b. Heaters 2–4 all have the same steady state load of just less than 3.5 kW. Each of these heaters are just recovering steady state losses from stacks and tanks in their stages. The load on tank 5 is almost double the loads on heaters 2-4 as it must recover energy lost in stacks in stages 5 and 6 as well as losses from tank 5.
7. HEAT TRANSPORT IN THE CONTACT LENS HYDRATION PROCESS

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
<th>Ref</th>
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</tr>
<tr>
<td>$T_2$</td>
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<td>°C</td>
<td></td>
</tr>
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<td>°C</td>
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</tr>
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<td>$T_4$</td>
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</tr>
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<td>1 min$^{-1}$</td>
<td></td>
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<td>$Q_1(10)$</td>
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<td>J kg$^{-1}$K$^{-1}$</td>
<td>[16]</td>
</tr>
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**Table 7.7**: Parameter values for cycle averaged model.
The biggest steady state demands are observed in the heaters in stage 1 and the preheat tank (heater 6). The estimate of the load in heater 6 should be more accurate compared to the other heaters as the uncertainty of the heat loss in the stacks is removed from the energy balance equation. The main load on heater 6 is to continuously heat PG entering at 81 min$^{-1}$ from 60$^\circ$C to 96$^\circ$C. Taking the largest values of specific heat capacity and density of PG over the range gives an upper bound for the power required. This gives a continuous power requirement of about 14.3 kW. Adding the tank losses gives a total power requirement of about 14.5 kW. This estimate should give a good upper bound for the power requirement during dosing. However before sizing heaters according to this, it is important to ensure that the incoming PG will be at 60$^\circ$C. If the incoming PG is at a lower temperature, an extra power requirement of 0.4 kW is required for each degree below this. Thus the 16.2 kW supplied by an 18 kW heater would not be sufficient if the entry temperature were 55$^\circ$C.

![Figure 7.23](image)

**Figure 7.23:** (a) Estimates of the average power demand on each heater in the production line. The heater size increments are marked on the vertical axis. Note the heaters can only deliver 90% of their rated power. (b) Breakdown of the energy requirements for each heater in the cycle averaged model.

The power requirement on heater 1 is almost 9 kW and thus appears too high for a 9 kW heater. The main power requirement is the load of heating two cold stacks. Given the conservative assumptions on the specific heat capacity of the trays, this is almost certainly overestimated. The steady state stack loss also likely overestimates the loss during heating of the stacks. However the model only supplies the cycle averaged demand and the first stage experiences a large
initial load when cold fluid first exits the stacks as was seen from the DI mini-stack experiments in section 7.3.1. Given such a load, it is important that the heater is sized to ensure that it can maintain the heater outlet temperature within the required tolerance. Thus the heater demand in stage 1 requires more careful consideration. Bearing in mind the desire to limit heater sizes to two options, these preliminary results suggest that heaters 1 and 6 require 18 kW heaters, while 9 kW should be sufficient for all other heaters.

7.4.3 Compartment model

The compartment model describing energy transport during the dosing cycle can be easily adapted to model the production line. As with the cycle averaged model, the volumes of compartments and flow paths and flow rates between compartments are changed to those in the production line system. The flow paths are shown in figures 7.21 and 7.22. The same parameter values as in the cycle averaged model, shown in table 7.7, are used. The control parameters for the PI controlled heaters are the same as those used on the mini-stack. The compartment model also has some extra parameters to be specified. The weir flow rate must be specified for each tank, as must the dosing flow rate from tank to stack. One of the total flow rate through the heater and the recirculation rate through the heater back into the tank must be specified. These flow rates are generally related through

\[ Q_2(i) = Q_3(i) + Q_4(i) \]

The flow rates and paths for \( Q_1(i) \) and \( Q_4(i) \) are shown in figures 7.24a and 7.24b. The total flow rate through the heaters \( Q_2(i) \) should be optimised to minimise heat loss. The minimum value required is that to meet the dosing flow rate \( Q_4 \) (or the refresh flow rate \( Q_1 \) for the preheat tank). Choosing these minimum values means there is no recirculation flow \( Q_3 = 0 \) to maintain tank temperature and all energy goes into heating the fluid going for dosing. The flow rate through the heaters can be set as high as 30 l min\(^{-1}\). If the dosing flow rate is 10 l min\(^{-1}\), the recirculation flow rate is 20 l min\(^{-1}\) and the heaters’ output is split in a ratio of 1:2 between the two flows. Maintaining a higher tank temperature has two main benefits. A higher temperature in the tank provides a buffer in the system to protect the heater from disturbances. For example, if tank 1 can be maintained at a temperature close to set point following the move time, the high tank temperature can absorb the initial shock of the cold exiting fluid, meaning the heater
7.4 Heater size estimates for production line hydration system

Figure 7.24: (a) Flow rates and paths during dosing in PG stages in production line system. (b) Flow rates and paths during dosing in DI stages in production line system.

As long as the peak demand time is sufficiently short, the heater can still reach the set point while the temperature of the tank drops slowly, absorbing the shock. The heater can then build up the tank energy again over the remaining part of the dosing cycle in preparation for the next shock. The second benefit is to maintain the energy in the refresh flow going from one tank to the next. For example, if heater 1 has a load near its capacity but heater 2 is only using 20% of its capacity, it makes sense to use more of heater 2’s capacity to heat the fluid in tank 2 and deliver the refresh flow from tank 2 to tank 1 at a higher temperature. The downside of maintaining tank temperature is a slightly higher loss from tank surfaces. Thus there is little point in maintaining the temperature of the preheat tank as the heater should be sized to continuously heat PG from the incoming temperature to the set point. Maintaining a higher tank temperature just increases the energy loss. Maintain-
ing tank temperature in tank 1 may also be counter productive. Apart from the possibility of absorbing a spike in demand, maintaining tank temperature in tank 1 means heating PG that is going directly to drain.

It is important to note that the compartment model assumes that all compartments are full and flow rates are constant throughout dosing. Thus the energy benefit to a tank from its neighbour through the refresh flow or conduction through the common tank walls may be exaggerated. This is important as each degree drop between tank $i$ and tank $i-1$ means a 0.39 kW power gain to tank $i-1$ from tank $i$ due to the refresh flow (of 81 min$^{-1}$). If the refresh flow is absent for some of the dosing time, and such a temperature difference exits between adjacent tanks, the demand on heater $i$ may be underestimated by the model. The energy benefit from conduction is comparatively small at 0.013 kW per degree difference between adjacent tanks. With reference to the results of the cycle averaged model, it seems optimal here to maintain tank temperature in tanks 2–4 where demand relatively low and thus maintain any benefit from the refresh flow to tank 1. The compartment model can be used to investigate this. Particular attention also needs to be paid to the influence of filling and emptying of stacks on the refresh flow and its implications for the load on heater 1.

The potential benefit of maintaining temperature in tanks mainly applies to the load on heater 1. The load here is large, but due to technical constraints the industry partner would like to ensure the heater is as small as possible. With this in mind we investigate the benefit of maintaining tank temperature in the PG tanks apart from the preheat tank (tanks 1-5). The flow rates to the stacks ($Q_4$) are fixed as in figure 7.24. The flow rate through heaters 1-5 is varied from 101 min$^{-1}$ to 201 min$^{-1}$. Thus the recirculation flow rate $Q_3$ is varied from 0 l min$^{-1}$ to 10 l min$^{-1}$ on these heaters. The resulting compartment temperatures and heater wattages are shown in figure 7.25 and 7.26. Note there is no recirculation on the preheat tank so it stays near the PG entry temperature of 60°C with only minimal loses from the tank surfaces. Looking at the wattage demand figures it can be seen that recirculation has a minimal effect on wattage demand on tanks 2-5. There is just a slight increase in demand, corresponding to the increased losses from the tanks. This is due to maintaining the tanks at a higher temperature. With tank recirculation of 101 min$^{-1}$ the temperatures of tanks 2-5 are approximately 3°C higher than with no recirculation. In stage 1 the effect of recirculation is quite pronounced. We can see that the instantaneous
and delivered wattage demand curves increase significantly for the first heater. Close inspection of the temperature curves reveals that the tank temperature in tank 1 does increase with recirculation and the lowest temperature reached in the tank is higher. However the lowest heater outlet temperature is actually lower. So recirculating in all tanks, as was the initial design intention, actually increased the power demand while delivering a worse result for the minimum temperature in tank 1.

![Temperature and Wattage Curves](image)

**Figure 7.25:** Comparison of the effect of maintaining tank temperature on stages 1–5. The temperature traces and heater wattage are shown for each simulation. The figures are labelled according to the simulation with the pair (total flow through the heater, recirculation flow back to tank). The final simulation is shown in figure 7.26.

The reason for the disimproved situation with recirculation is two-fold. Imparting a benefit from tank to tank relies on a temperature differential between
Figure 7.26: Plots for final simulation from figure 7.25

tanks, thus recirculation on tank 1 is a negative from this view-point. Main-
taining temperature on tank 1 is desirable to insulate against the shock to the
system of the cold stack entering, and it does maintain a higher tank tempera-
ture. However, when the shock does come, if the flow rate is 20 l min\(^{-1}\) instead
of 10 l min\(^{-1}\), the heater can only recover half the temperature drop and so the
actual outlet temperature is lower for this period. The fact that at 20 l min\(^{-1}\) the
heater gives equal priority to maintaining tank temperature and temperature of
fluid being transferred to the stack means a higher power requirement and worse
results in terms of the key heater outlet temperature. Thus the solution is to
remove recirculation on tank 1 and allow the increased benefit from tank 2 to
maintain tank temperature, while heater 1 fully prioritises its outlet temperature
of fluid to the stack. This situation is simulated in figure 7.27. It can be seen that
the power requirement on heater 1 in this case is lower than any of the three con-
figurations in figures 7.25 and 7.26, while the lowest outlet temperature reached
is actually higher. Thus this configuration is considered optimal. Considering
figure 7.27b the earlier suggestion that heaters 1 and 6 require 18 kW heaters,
while 9 kW should be sufficient for all other heaters remains the best recommen-
dation. The model has also been extended to include the different flows during
backflush and move time (without modelling compartment volume change). As
results do not change significantly they are not presented here. However the in-
dustry partner would like some further investigation on the viability of placing a
9 kW heater on stage 1. Specifically it is of interest to investigate the minimum
outlet temperature reached during a typical cycle in stage 1 if a 9 kW heater is in place.

![Temperature and wattage plots](image)

**Figure 7.27:** Temperature and wattage plots for maintaining tank temperature on tanks 2–5 but not on tank 1.

### 7.4.4 Modelling energy demand in stage 1

The industry partner is interested in the implications using a 9 kW heater on stage 1, in terms of the heater outlet temperature. The compartment model above suggests that the refresh flow through the hydration system can be leveraged to supply additional energy to stage 1 by maintaining the temperature on upstream tanks. This would serve to reduce the load on heater 1. However we need to be careful to consider some of the assumptions of the model. It is assumed that the weiring flow from tank to tank occurs through the full dosing cycle. This will not be the case as at least some emptying of stacks occurs during move time. Thus during the initial phase of each dosing cycle, some time passes while the stacks refill, before the weiring flow is established. The biggest load on heater 1 occurs about 60 s into the dosing cycle (or soon after depending on tank 1 temperature) when the first cold PG exits the stack in stage 1. If the weiring flow is not established by this point, it will not be of any benefit in preventing the lowest heater outlet temperature. Thus before looking in detail at the energy balances in stage 1, it is important to consider the volume changes in compartments during a dosing cycle.
Ignoring the preheat tank, the PG system has 5 tanks with a capacity of 30 l each. Each of these must be full for any weir flow to take place from them. Each stage has 2 stacks, which experiments estimate contain 5 l each at steady state. It is estimated that when the stacks empty they contain 2.5 l each. If we assume the worse case, than during the move time each of these stacks’ fluid volume reduces from 5 l to 2.5 l and this fluid overflows from tanks to tank and leaves the system. Thus 30 l may be lost from the system during move time. When dosing begins all tanks are full, but the stacks in stage 1 are empty and the stacks in stages 2–6 are half full. To fill the stacks initially the volume of tanks starts to drop. The stacks in stages 2–6 will be full in 30 s while it will take 60 s in stage 1. Thus without the refresh flow the volume of tanks in stages 2–5 will be 25 l and 20 l in stage 1. The refresh flow is 8 l min$^{-1}$ and will refill the tanks consecutively starting with tank 5 after it has filled the stacks in stage 6. Before any weir benefit is imparted to stage 1, 25 l must be delivered to the system. This takes 187.5 s or 127.5 s after fluid has begun to exit stacks into stage 1. Thus we cannot assume that the weir flow has any benefit to the temperature in tank 1 during the part of the dosing cycle when heater 1 experiences the largest demand.

As stage 1 may essentially operate in isolation from the other stages for about 3 minutes of a dosing cycle, and any possible interaction should be positive from an energy viewpoint, we can model the energy transport in stage 1 independently from the other stages. To simplify the model, we use the temperature drop data from the single stack experiment to estimate the temperature of the fluid exiting the stack. Assuming the same energy loss we extrapolate the temperature drop data for water to generate a temperature drop time series for PG. Using a set point temperature of 96°C we can estimate the exiting temperature of PG from the stack. The extrapolated data is fitted with a function of the form $T_{exit}(t) = a - be^{-ct}$ where $t$ is the time since fluid first started to exit and $a$, $b$ and $c$ are constants. The fitted function and data is shown in figure 7.28.

With this data we can now define a differential equation for the tank temperature in stage 1 over the first few minutes after fluid begins to exit stack 1. This will give us a prediction of the demand on heater 1 over this period. We make the following assumptions:

- The empty stacks fill in 1 minute.
7.4 Heater size estimates for production line hydration system

![Graph showing exit temperature of PG fluid from stacks against time]

Figure 7.28: Exiting temperature of PG fluid from stacks in stage one plotted against the time since fluid began to exit stacks. Data points are extrapolated from single stack experiment with water and fitted with the function $T_{exit}(t) = 90.4136 - 63.31668e^{-0.0224878t}$.

- Once the stacks are full the tank has 20 l of PG at a known temperature.
- The fluid in the tank is well-mixed (uniform tank temperature).
- There is no weir effect for at least the next 2 minutes, so no volume change.
- We denote time $t = 0$, as the time fluid starts to exit the stack and enter the tank. We denote the tank temperature at this point $T_0$.
- We have the exiting PG temperature from the stack as a function of time (described above).
- There are no control delays, heater demand given will be instantaneous demand to reach set point of 96°C.
- Energy transfers in tank accounted for are:
  - Loss in energy of $101\text{min}^{-1}$ PG at tank temperature.
  - Gain in energy of $101\text{min}^{-1}$ PG exiting stack at given temp.
  - Loss of energy from tank walls to air.
Conduction from tank 2 is ignored.

- Note there is no feedback in model. The exiting temperature data is used even if temperature doesn’t hit set point.

The energy balance equation for the tank in stage 1 is now defined as

\[ V_d \rho_p c_p^* \frac{dT_d}{dt} = Q_4 \rho_p c_p^* (T_{exit} - T_d) - h_{d,air} A_{d,air} (T_d - T_{RM}). \]  

(7.4.12)

Rearranging we get

\[ \frac{dT_d}{dt} = \frac{Q_4}{V_d} \left( T_{exit} - T_d - \frac{h_{d,air} A_{d,air}}{Q_4 \rho_p c_p^*} (T_d - T_{RM}) \right), \]  

(7.4.13)

with

\[ T_{exit}(t) = a - be^{-ct}, \]  

(7.4.14)

and

\[ T_d(0) = T_0. \]  

(7.4.15)

This equation can be solved exactly for the tank temperature as a function of time. The initial tank temperature in the tank is not known exactly but is likely around the exiting temperature of exiting fluid from stacks at steady state. Data suggests this may be around 90°C. To allow for the uncertainty in this value we consider a number of initial temperatures around this value.

We recall from equation (7.2.10) that the maximum temperature difference that a heater with maximum wattage \( W_{\text{max}} \) can recover is given by

\[ \Delta T = \frac{W_{\text{max}}}{Q_2 \rho c^*}. \]  

(7.4.16)

A 9 kW indirect heater can deliver at most 8.1 kW and so for PG with a flow rate of 10 l min\(^{-1}\) it can make up about a 16.5°C temperature drop. Thus if the tank temperature drops below 79.5°C the set point cannot be reached. Figure 7.29a shows the solution to (7.4.13) for a range of initial temperatures from 85°C to 92°C. The tank temperature can be seen dropping significantly in the first minute after fluid starts to exit the stacks. It is clear that the tank temperature drops below 79.5°C in all cases. As the stacks heat up the exiting fluid temperature rises and eventually is greater than the tank temperature again so that the tank temperature rises again. Based on the discussions above all this happens in the
time window where there may be no weir flow from tank 2. The instantaneous wattage demand is shown in figure 7.29b. We can see that the maximum heater capacity is exceeded in all cases. In figure 7.30a the time during which the power requirement is above capacity is plotted as a function of the initial tank temperature. The process specifications require the heater outlet temperature to be within 2°C of the set point at all times. Figure 7.30b shows the actual heater outlet temperatures that can be achieved in this case (assuming ideal heater operation). Thus based on the model simulations, a 9 kW heater is unlikely to be sufficient to maintain the heater outlet temperature within process specifications in stage 1. Unless the process requirements are adapted to allow for a period outside these specifications a larger heater is recommended.

Figure 7.29: (a) Tank temperature in stage 1 for different initial tank temperatures. (b) Wattage demand on heater 1 to achieve set point for different initial tank temperatures. Maximum capacity of a 9 kW heater is marked.

Figure 7.30: (a) Time during which the power requirement on heater 1 is greater than capacity of a 9 kW heater for different initial tank temperatures. (b) Heater outlet temperatures that can be achieved with a 9 kW heater based on tank temperatures in figure 7.29a.
7. HEAT TRANSPORT IN THE CONTACT LENS HYDRATION PROCESS

7.5 Conclusions

In this chapter, the sizing of heaters for the production line hydration process outlined in chapter 6 was considered. Given the complex nature of the process involved and the comparatively limited amount of experimental data available, the models used to simulate the process were energy balance models, focusing on the macroscale transfers of energy in the system. These models divide the hydration system into a number of compartments and model the transfer of energy within and between the compartments. The temperature of each compartment is a key output of the models. The models used are based on simplifying assumptions, such as well-mixed compartments, which reduces the set of parameters which have to be estimated from experimental data. The aim was to estimate how much energy is lost in each stage in the process, during a dosing cycle and thus how much energy needs to be supplied by the heating units in the system. These predictions allow the heaters to be sized to meet the system demands.

The main models used were a cycle averaged heat transport model and a time dependent heat transport model. The cycle averaged heat transport model estimates the average heater load in each stage over a dosing cycle. The model provides a quick estimate of approximate heater loads in each stage and gives a good reference with which to compare more sophisticated models. The model was fitted and compared with available data from the mini-stack rig apparatus. The time dependent heat transport model gives an estimate of the demand on each heater during a dosing cycle. Heaters in the hydration system operate in order to keep their outlet temperature at a fixed set point. Heater operation is determined by a PI controller, based on the set point error and the history of set point errors. In order to replicate experimental data, simulation of the PI controller is incorporated into the model. The model is fitted and compared with available data from experiments and some undesirable controller behaviour is investigated and explained.

Following investigation and parametrisation of the models with the experimental data, the model parameters and equations were altered to describe the production line hydration process. Based on the model simulations, taking into account the desire for just two different heater sizes and a reasonable cold start-up time, the following recommendations are made:

- The models indicate that 9 kW heaters are sufficient on tanks 2-5 and 7-9.
7.5 Conclusions

- An 18 kW heater is required on the pre-heat tank. Care should be taken to ensure that the entering PG is at 60°C and not any lower. If the entry temperature is 55°C or lower then an 18 kW heater is insufficient.

- An 18 kW heater is required in the first stage, as a 9 kW heater may lead to a drop in the outlet temperature outside the process specifications.

Some further points are worth noting:

- Due to limited data, especially relating to PG dosing, a number of parameters had to be estimated. Where this was the case, estimates were conservative and chosen to overestimate, rather than underestimate heater sizing.

- Examples of this include the overestimation of specific heat capacity for Ultem and not accounting for the fact that the production line apparatus is in an enclosed environment, likely to be well above room temperature.

- Heat losses from system plumbing and shower-heads were not explicitly included in the model but may be hidden in some of the fitting parameters. In any case, the single stack experiment showed that these losses may be significant and so the system plumbing and shower-heads should be insulated on the production line model.

- The recommendation to maintain tank temperature on tanks 2-5 is still valid, but its benefit should be further investigated if more information becomes available on the exact details of the weiring flow during dosing.
7. HEAT TRANSPORT IN THE CONTACT LENS HYDRATION PROCESS
8.1 Introduction

The primary function of the hydration process outlined in chapter 6 is the leaching of unwanted material from the cured and moulded lenses. The lenses under consideration here contain a component called 3,7-dimethyl-3-octanol (D3O), which is insoluble in water, so hydration is a two-step extraction. Initially, an organic solvent called propylene glycol (PG) is used to remove the D3O, before deionised water (DI) is used to remove the PG. In the first step the lenses are contacted with PG. The PG infiltrates into the dry polymer lens, causing the polymer matrix of the lens to swell and providing a medium through which the D3O can be leached from the lens. The D3O dissolves into the PG in the lens and diffuses out of the lens, driven by the concentration gradient between the D3O in the PG in the lens and the PG surrounding the lens. The particular set-up of the hydration apparatus developed by Vistakon aims to maximise the concentration gradient throughout extraction. Fresh PG solvent is introduced into the system at a fixed rate to maintain the concentration gradient, while contaminated PG is removed at the same rate. To ensure all lenses are extracted properly, the concen-
tration gradient between the lenses and the hydration fluid should be maintained as large as possible so as not to limit extraction and a sufficient total extraction time must be given for diffusion to occur from the lens. If the process is temperature sensitive and there is a temperature variation in the hydration fluid in a stack, process specifications should be chosen to cater for the lens with the least favourable conditions. A secondary consideration, is that the PG extraction time should be large enough to allow lens release. This time may be larger than that required for chemical extraction from the lens.

In the second step the lenses are contacted with DI. DI and PG are fully miscible so the DI diffuses into the lens mixing with the PG while the PG diffuses out. The concentration gradient between the hydration fluid (in this case DI) and the PG in the lens is maintained by delivering DI into the system at a constant rate and removing DI contaminated with PG. During this process the volume of the lens decreases, as the equilibrium volume of a water saturated lens is much lower than that for a PG soaked lens. This process is thought to be less temperature sensitive, but again sufficient time must be allowed for the PG to be extracted from the lens which has the least favourable conditions.

In this chapter, we will begin by presenting a number of experiments which investigate the process parameters and configurations necessary to achieve complete extraction of D3O and PG from the lenses. Complete extraction here means that the final lens must contain less than 200 ppm mass of D3O or PG per mass of dry lens. The experiments are conducted on the mini-stack rig and investigate the influence of process variables such as the total extraction time, refresh flow rate to the system and process temperature. Certain conclusions were arrived at which informed the design of the production line hydration system. Despite this, there are a number of key questions concerning the extraction in the hydration system and the optimum system parameters which will make the process as efficient as possible, while minimising its cost.

8.1.1 Key questions

The key questions regarding the chemical extraction in the hydration system are:

1. Influence of a blocked nozzle on concentration of D3O in the final lens: If a nozzle gets blocked, in one of the shower heads, in one of the washings stages in the system, will the final lens still be within specification?
2. What concentration of D3O in the incoming PG, will still result in a fully cleaned lens? Tests performed by the industrial partner show that PG distilled to have 5 ppm D3O concentration does not significantly impact the extraction efficiency. The question is: will higher D3O concentrations be as effective/effective enough? This is relevant, as it may allow the reuse of PG in the system. The distillation of PG to low concentrations of D3O is also an expensive process, so it is useful to determine the critical level of D3O concentration in the solvent which still allows effective cleaning of the lenses. A related question is how the efficiency of PG as a cleaning medium is reduced when it is diluted with D3O as it moves through the system.

3. What is the optimum stack height to ensure all lenses are sufficiently cleaned? It is observed that the lenses at the top of stacks are cleaned more effectively than the lenses at the bottom. It is felt that this is related to the temperature drop in PG solvent in a stack from top to bottom, rather than purely being reduced extraction due to the accumulation of D3O in the PG solvent, as it cascades down through the stack, causing a smaller concentration gradient at the bottom. Increasing the stack height (for a fixed inflow rate) results in a larger drop in temperature between the top and the bottom and also potentially a temperature drop between the centre and edge positions in the trays which becomes more pronounced lower down in the stack. Thus if temperature drop is the cause of this reduced extraction rate from top to bottom, an equivalent question is to ask how does temperature influence the extraction rate of D3O?

4. Similar questions may need to be addressed in relation to extraction of PG with water.

**8.1.2 Modelling challenges**

The hydration process under consideration is a very complex operation. We will focus here on the extraction of D3O from the lenses. The details for extraction of PG with DI are similar. The chemical extraction of D3O from the lenses consists of a number of steps which will need to be modelled. Before considering the available experimental data we discuss some of the modelling challenges which need to be overcome.
8. CHEMICAL TRANSPORT IN THE CONTACT LENS HYDRATION PROCESS

8.1.2.1 Initial extraction period

Initially the PG must infiltrate the dry contact lenses and dissolve the D3O contained in the lenses. This process is complicated by a number of issues. The incoming lenses and the stack which contains them are at room temperature as discussed in chapter 7. Thus during the initial dosing period the stack and lenses are getting up to temperature. This will happen much quicker at the top of the stack. It is unclear how this initial non-isothermal period affects the dynamics of PG infiltration and initial extraction. Furthermore during this period the lenses are swelling. It is clear that the D3O extraction rate is likely to be uneven in this period. As the porosity in the lenses increases, more PG can infiltrate into the lenses which may decrease the D3O concentration in the PG in the lenses thus tending to decrease the concentration gradient between the PG in the lenses and the surrounding PG solvent. In the meantime, the average diffusion distance from the lenses to the bulk PG fluid is increasing and the temperature is increasing. It is clear that this initial period in the process cannot be modelled accurately, without detailed experimental insights and data on this period to inform any modelling.

An alternative to modelling the initial period, is to obtain data for the D3O lens concentration following this period and assume the process is then isothermal, and the lenses have swelled to their equilibrium state. During this isothermal extraction period the extraction rate should be far more predictable. Neglecting modelling the initial extraction period has a number of draw backs. The initial extraction is likely to extract the lenses at the top to a greater extent, this difference needs to be determined experimentally. Also, without some description of this initial extraction period, it will be difficult develop a model which can reliably describe changes to process variables which affect the dynamics of this initial extraction period.

8.1.2.2 Isothermal extraction period

Once the lenses have reached their equilibrium PG content and temperature, the extraction should be more well behaved. There will be a steady temperature drop from the top of the stack to the bottom which will depend on the volume flow rate to the stack. This may lead to a difference in the extraction rates in these locations. For sufficiently low volume flow rates, a temperature drop is also likely
to be evident from the centre positions in the trays to the edges. This drop will increase from a value close to zero at the top tray and may be significant at lower flow rates. The D3O concentration in the PG solvent will increase as the PG flows down through the stack. If this increase in concentration is sufficient to decrease the concentration gradient between the lenses and the solvent significantly, this may lead to reduced extraction in the trays lower in the stack. This difference in lens D3O concentration based on position in the stack, can be identified as significant in data from extraction experiments. Further investigation is needed to decide if this is due to a reduced concentration gradient, a reduced diffusion rate due to a reduced temperature or a pre-existing difference from the initial non-isothermal extraction period.

The dynamics of the fluid, which cascades over the lenses down through a stack, is complicated and would be extremely difficult to model accurately. While the nature of the flow will influence the extraction rate, no attempt will be made to model it here. Instead we will use simpler models to track the transport of D3O in the system. These models will have certain parameters which need to be fitted from experiment. A certain amount of data is available from testing on the mini-stack rig, a scaled down version of the production line. Any unknown parameters in our models must be fitted by comparison to data from the mini-stack rig.

Where the model parameters depend on temperature, flow rates etc. the nature of this dependence must be found from the mini-stack rig experiments in order to apply the model to the production line set-up, where temperature and flow rates may be different. In particular, the effective rate of diffusion of D3O from the lenses will likely depend on the temperature of the lenses, velocity and viscosity (which also depends on temperature) of the solvent flowing over the lenses and the porosity of the lenses (i.e. the volume fraction of the solvent in the lenses). However this effective diffusivity will just be determined by fitting experimental data. If the models need to be extrapolated to different process parameters then the nature of any dependence of the effective diffusivity (or other model parameters) on the process parameters needs to be determined from experiment. Thus potentially important parameters for extrapolation to the production line, such as temperature, need to be varied independently from other parameters during experiments.
8. CHEMICAL TRANSPORT IN THE CONTACT LENS HYDRATION PROCESS

8.1.3 Modelling strategy

The modelling strategy will be to formulate a series of models of increasing complexity, to describe the extraction and transport of D3O and PG within the hydration system. The models will be parametrised by fitting concentration data from the mini-stack rig experiments. The effectiveness of any model in describing extraction will be assessed from the quality of the fit. Unless the process is dominated by noise it is quite likely that a model can be chosen to fit the experimental data. Care must be taken to ensure that the model captures the physical behaviour of the system rather than just describing a particular experimental set-up. This is a key requirement for the model to be valid for different sets of parameters.

8.2 Experimental data

Experimental data on concentrations of D3O and PG in lenses following hydration for different process parameters on the mini-stack rig is available. The data on lens concentration is collected after the lenses have gone through all five stages of the mini-stack rig. Lens concentration data is collected for lenses in both the top and bottom positions in the stack at the stack centre and edges. Some limited data is available for the D3O concentrations in lenses following the first and second PG extraction stages. In these instances PG extraction was conducted in the first stage (for example) but subsequent stages 2 and 3 were skipped before the PG is extracted with DI in stages 4 and 5. These experimental runs are called the deconstruct samples. According to the industry collaborator once PG extraction is over, no further D3O is extracted from the lenses. If this is the case, D3O data from deconstruct samples should give reliable data on the D3O concentration after stages 1 and 2. Deconstruct samples are only available for the top centre and top edge positions. Experiments were conducted under two different set-ups of the flow paths in the mini-stack rig. We refer to these set-ups as the March and June set-ups. The set-ups differ in how fresh PG and DI are delivered to the system as shown in figure 8.1.

The March experiments compare different extraction times and different dosing rates. The effective dosing rate is defined as the volume of fresh PG added in an index time, divided by the number of lenses in a stack and is given in
(ml/lens). Following on from the March experiments, a proposed process with a PG extraction time of 2700 s and a DI extraction time of 1800 s with an effective dose rate of approximately 8 ml/lens was assessed in the June experiments. Fresh solvent was delivered to the top of the stack in last stage rather than to the tank.

A statistical analysis of this data has been undertaken and is documented in a separate report for the industry partner. In this exposition we will just present the key findings relevant to the model development. The variation in D3O concentration based on position is found to be statistically significant. D3O concentration is higher in lenses at the bottom of the stacks than at the top. D3O concentration is also higher in lenses at the bottom edge than the bottom centre. The data points are found to be fitted reasonably well using an exponential decay rate, within the range of extraction times covered. However, extrapolation of this formula to infer the initial condition, shows that the extraction rate must be much higher during the initial stage than over the rest of the extraction time. No data is available to investigate the dynamics of extraction during the initial period. Also, as there is no deconstruct samples for the bottom lenses, we cannot infer if the positional effects are established during the initial non-isothermal extraction period or as the result of a difference in extraction rate during the rest of the extraction (or a combination of both).

For PG removal with DI, the difference between the concentrations in lenses at the top and bottom of the stacks is also identified. However the data is too variable to be correlated with DI extraction time. Thus as the extraction mechanism is unclear from the data it will not be possible to model PG extraction accurately without further data or insight into the extraction process.

8.2.1 Motivation for choosing models: D3O data

The structure of the experiments does not allow us to find correlations between the final concentrations and temperatures, flow rates, stack heights etc. To consider what models are appropriate to describe the D3O extraction we consider the experiments which are closest to the production line set-up. These are 3 trials from the June experiments which have index times of 600 s, 750 s and 900 s and flow rates as indicated in figure 8.1a. The weir flow rate is varied from the listed 11min$^{-1}$ to keep the effective dose approximately constant.
Thus we have experiments with PG extraction times of 1800 s, 2250 s and 2700 s. Following PG and DI extraction, lenses from different positions in the stack are sampled and their D3O concentration is measured. Concentration is measured in mass of D3O per mass of dry lens in parts per million (ppm). Each experiment is replicated three times to assess any variations in results. Thus, while noting that experimental conditions may be slightly different, we have D3O concentration data at three different time points at centre and edge positions at the top and bottom of the stacks. As well as this, for each experimental index time deconstruct runs were performed, where PG dosing only occurred at the first or the first and second stages. These stacks were then run through the DI stages and concentration of D3O was measured, but only in the top tray at centre and edge positions. These experiments were not replicated so we cannot assess any random experimental affects. The experiments do however give extra data for D3O concentration at the times 600 s, 750 s, 900 s, 1200 s, 1500 s and 1800 s.

### 8.2.1.1 Exponential decay

To begin, we ignore positional influence and just plot all D3O concentration data against time in figure 8.2a to identify general trends. Noting it looks like the data may be fitted with an exponentially decaying function, we look at the plot on a log-scale. It is clear that, while the data is quite variable, the points can be fitted with a line of negative slope. Thus the experimental data for D3O concentrations in ppm is quite well described by a function of the form

\[
c_{D3O} = ae^{-bt} \tag{8.2.1}
\]
8.2 Experimental data

![Image](image_url)

**Figure 8.2:** (a) D3O concentrations in ppm mass D3O per mass dry lens. (b) Plot of data on a log-scale. Initial value is included. (c) Fit of the function $ae^{-bt}$ to the data plotted on a log-scale. (d) Fit of the function $ae^{-bt}$ to the data.

with $a$ and $b$ constants. Fits of this function to the data are shown in figures 8.2c and 8.2d.

This suggests that even without considering the increase in concentration of D3O in the PG fluid as it flows through the system, the lens D3O concentration can be reasonably well modelled by the differential equation

$$\frac{dc_{D3O}}{dt} = -bc_{D3O}, \quad (8.2.2)$$

with initial condition

$$c_{D3O}(0) = a, \quad (8.2.3)$$

where $a$ is the initial concentration of D3O in the lenses and $b$ is the extraction rate. Unfortunately extrapolation of the fitted exponential formula to estimate the initial concentration in the lenses gives an initial condition which is less than one tenth the value of the real initial concentration of D3O in the lenses, which is 230000 ppm. This value is plotted in the log-scale plots for comparison. It
is also evident that the fitted extraction model underestimates the deconstruct concentration measurements. It is unwise to read too much into this as the deconstruct measurements were not replicated and are subject to greater uncertainty than the other measurements. However, it is clear that the rate of change of D3O concentration is much faster during the initial phase of extraction before becoming approximately proportional to the concentration of D3O for the time period covered by experimental data collected here. It should be noted that the concentration as measured here, is just a proxy for mass of D3O in the lens. It does not represent the actual concentration of D3O in the PG in the lens pores which will vary significantly (at least initially due to PG infiltration and lens swelling).

### 8.2.1.2 Fast-slow D3O extraction

It is quite easy to fit the observed data and initial condition by introducing extra degrees of freedom into the fitting equations. One way to do this is to split the D3O mass into two (or more) groups which extract at different rates. For example we can fit the data by a function of the form

$$c_{D3O}(t) = c_{fast0}e^{-r_1t} + c_{slow0}e^{-r_2t}, \quad (8.2.4)$$

where $c_{fast0} + c_{slow0} = 230000$. The constant $c_{fast0}$ represents the concentration of fast extracting D3O while $c_{slow0}$ represents the initial concentration of slow extracting D3O. The best fit of this function to the data with $c_{fast0} \approx 214000$, $c_{slow0} \approx 16000$, $r_1 \approx 0.00874$ and $r_1 \approx 0.0019055$ is shown in figure 8.3a. This formula corresponds to modelling the extraction of D3O from the lenses with differential equations of the form

$$\frac{dc_{fast}}{dt} = -r_1 c_{fast}, \quad (8.2.5)$$

$$\frac{dc_{slow}}{dt} = -r_2 c_{slow}, \quad (8.2.6)$$

with

$$c_{fast}(0) = c_{fast0}, \quad c_{slow}(0) = c_{slow0}. \quad (8.2.7)$$

The D3O concentration is given by $c_{D3O}(t) = c_{fast}(t) + c_{slow}(t)$. 

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8.2 Experimental data

8.2.1.3 Time-dependent extraction rate

A second option is to define a time dependent extraction rate. This rate can be piecewise defined (e.g. for different stages) or continuous. As an example the function

\[ c_{D3O}(t) = c_0 e^{-b(t)t}, \]  

(8.2.8)

with \( c_0 = 230000 \) and \( b(t) = r_1 + r_2 e^{-r_3 \sqrt{t}} \) can be fitted to the D3O data as shown in figure 8.3b. This corresponds to modelling extraction of D3O from the lenses with a differential equation of the form

\[ \frac{dc_{D3O}}{dt} = -\tilde{b}(t)c_{D3O}, \]  

(8.2.9)

with initial condition

\[ c_{D3O}(0) = c_0, \]  

(8.2.10)

where \( c_0 = 230000 \) and \( \tilde{b}(t) \) is a time dependent extraction rate. The function \( \tilde{b}(t) \) is to take account of changes in the extraction rate during the initial non-isothermal extraction period in the first stage. As there is no data for lens concentrations in the early extraction period it is easy to pick a function which will ‘fit’ a particular experiment. However this function may not describe extraction well for changes in parameters. In reality \( \tilde{b}(t) \) probably depends on variables such as lens volume and temperature. Identification of this dependence is impossible without experimental data on these variables.
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8.2.2 Positional influence: D3O data

As mentioned earlier, D3O concentration is found to correlate with position in the stack. For illustrative purposes, we just divide the points by vertical position (i.e. top or bottom). The data is plotted in figure 8.4a. It is clear that, on average, the D3O concentrations are higher at the bottom than the top. However, it should be noted there is significant variability in the measurements. Even from the same experimental realisation there are examples where the concentration at a bottom position is lower than that at a top position. The source of this variability is not clear. Figure 8.4b shows the fit of an exponentially decaying function to available data at the top and the bottom. The comparison appears to show a faster decay rate at the top, however this is not a valid comparison as no deconstruct data is available for the bottom position. Figures 8.4c and 8.4d show the comparison without the deconstruct points. Here the extraction rates are broadly similar and the fit suggests that the differing concentrations may be due to an uneven extraction during the initial non-isothermal extraction in the first stage. This is however just speculation. What is clear is that without deconstruct data for the bottom tray we cannot be certain whether the differing concentration at the bottom is due to a reduced extraction over the whole process or a difference established within the first stage or both. It could also be argued that the data suggests that the low flow rate of 1 l min$^{-1}$ in the last stage may lead to a slower extraction rate which may emphasise the difference between the top and bottom positions. However this is not clear. It is possible that the temperature drop in the stack is the factor determining the concentration difference between the lenses in the top tray and the bottom tray. However it is difficult to quantify this with the data available. As has been mentioned, some consideration should also be given to ascertain whether the concentration difference in the PG solvent entering and exiting a stack is significant enough to influence the extraction rate in trays lower down in the stack.

While positional variation in extraction is clear from the data, it will difficult to fit different extractions rates for different positions without at least having some data at earlier times for the bottom tray positions. Reliable correlations of extraction rate with temperature would further require variation of temperature independent of other process variables.
8.2 Experimental data

Figure 8.4: (a) Data points divided by position (top or bottom) in stack. (b) Data fitted with exponentially decaying functions. (c) Data with deconstruct points removed. (d) Data with deconstruct points removed fitted with exponentially decaying functions.

8.2.3 Basic modelling conclusions: D3O data

The key component of a model of the hydration process is an accurate representation of the extraction kinetics from an individual lens. The parameters of this model can be made dependent on lens position, lens porosity, temperature and the properties of bulk extracting PG in contact with the lens, where physical mechanisms can be established or correlations can be established. Based on the observations from experimental data we outline some models for extraction for a single lens that can serve as building blocks for modelling the full system.

8.2.3.1 Isothermal extraction from a lens

Once the initial non-isothermal extraction period is over and the temperature distribution in the stacks has reached steady state, it appears extraction from a lens can be described by a constant extraction rate. During this period we assume that the PG has infiltrated the lens and mixed with the D3O inside. As the PG
fluid is continuously flowing over the lens surface it seems reasonable to assume
the major resistance to extraction is diffusion of D3O from the lens rather than
resistance to entering the bulk fluid. We assume that the rate of change of D3O
mass in the lens is proportional to the difference in concentration of D3O in the
lens and the bulk PG fluid:

\[
\frac{dVlc_l}{dt} = -\frac{D_l A_l}{r_l} (c_l - c_{PG}),
\]
(8.2.11)

where \(V_l\) is the volume of solvent (PG) and solute (D3O) in the lens, \(c_l\) is the
concentration of D3O in the lens (mass per unit volume), \(c_{PG}\) is the concentration
of D3O in the bulk PG fluid (mass per unit volume), \(D_l\) is the diffusion coefficient,
\(A_l\) is the external lens surface area exposed to PG solvent and \(r_l\) is measure of
the diffusion distance from the lens interior to the bulk fluid. The experimentally
measured concentrations are given as mass of D3O per mass of dry lens in ppm.
As the mass of the dry lens is fixed, we essentially have measurements of the
mass of D3O in the lens at given times. Thus the fact that we can fit the rate of
decrease of concentration in ppm as being proportional to itself suggests that the
volume of PG in the lens is approximately constant during the period over which
the data was collected. So the assumption of constant volume seems reasonable
for this period. In this case the rate of change of concentration in a lens can be
written as

\[
\frac{dc_l}{dt} = -\frac{D_l A_l}{V_l r_l} (c_l - c_{PG}),
\]
(8.2.12)

It is important to note that using the correct final volume for PG in the lens
is important to determine final mass of D3O in the lens. The model has an
equilibrium when \(c_l = c_{PG}\). Suppose the volume of PG in the lens we use is twice
the actual volume. The equilibrium mass in the lens is then twice its actual value
and so is the mass concentration of D3O per mass of dry lens. This is particularly
important if we want to assess the ability of initially contaminated PG to clean
the lenses. So, for example, a 50 ppm D3O concentration in the incoming PG
should at best lead to an equilibrium concentration of 50 ppm in the PG in the
lens. The correct volume is needed to find the D3O mass in the lens and thus the
corresponding mass concentration of D3O per mass of dry lens. The equation can
also be easily rewritten in terms of the concentration units of the experiments,
by use of a partition coefficient to represent the equilibrium state between the
concentration (mass D3O per mass dry lens) in the lenses and the concentration (mass D3O per volume PG) in the PG solvent.

The diffusion coefficient $D_l$ can be made dependent on temperature, PG flow rate, etc., for lenses in different positions in the system but only if such correlations can be established.

8.2.3.2 Non-isothermal extraction from a lens

It is clear from the data that the majority of D3O is extracted in the first stage and within the first 600 s. We have referred to this as the non-isothermal period of extraction, but the process is very dynamic during this period and a number of processes other than just temperature variation are ongoing. The PG infiltrates the lens and mixes with the D3O. The lens pores also swell significantly during this period. All these processes may be temperature dependent. As the fluid must heat the cold stack initially, the temperature in the bottom trays lags below the temperature at the top for some time. Available data for linear volume swelling percentages at equilibrium suggest that the volume of the lenses may increase by as much as 50% in PG. This could mean a doubling of the initial pore volume in the lenses. This would clearly serve to reduce the concentration difference between D3O in the PG in the lenses and D3O in the bulk PG. However we have limited understanding of either the physics of extraction in this period or the chemistry involved. There is also no data for this period. Thus attempting to model the physics of extraction in this period doesn’t seem feasible.

We have already shown that two alternative approaches can be used to fit the data and initial condition. These can be motivated by volume or temperature changes. The first is to separate the D3O mass in a lens into two different groups which extract at different rates. The mass assigned to each group and extraction rates must be fitted to data. The extraction from each group will be governed by an equation similar to equation (8.2.12). The second option is to define a time dependent diffusion coefficient which approaches the fitted diffusion coefficient for the isothermal extraction over the initial transient period. For example $D_l$ in equation (8.2.12) could be defined as

$$D_l = D_0 + (D_\infty - D_0)(1 - e^{-kt}),$$

(8.2.13)
Figure 8.5: (a) Final PG concentrations in lenses following hydration (June data). (b) Final PG concentrations in lenses following hydration on log-scale (June data).

where $D_0$ is the initial diffusion coefficient and $D_\infty$ is the diffusion coefficient during the isothermal extraction period. The constant $k$ defines the timescale over which $D_l$ decreases from $D_0$ to $D_\infty$. Again $D_l$ can be defined to depend on temperature directly or via position and time dependence.

### 8.2.4 PG concentration data

The PG data for both the March and June experiments is highly variable. It is difficult to discern anything about the extraction of PG with DI water from it. Data from the June experiments is shown in figure 8.5.

### 8.2.5 Lens geometry

The geometry of the lenses being hydrated is important to determine the volume, cross-sectional area and thickness of the lens, key parameters which will influence extraction. The lenses used are 12.00D/8.5mm lenses which have a final diameter of 14.3mm and a base curve radius of 8.5mm. The power of the lenses is 12 dioptres. The base curve (back) of the lens is formed by a section of a sphere or spherical cap, a cross-section of which is shown in figure 8.6. The base curve radius is half the length along the minor arc between the two endpoints of the cross section of the lens as shown. The lens diameter is the diameter of the circular base of the spherical cap. The perpendicular distance from the diameter line to the apex of the base curve (the sagitta) is 3.8mm. Other geometrical properties such as the angle subtended by the arc and the radius of the sphere defining the lens can be easily calculated. The shape of the front curve of the lens
determines the power of the lens. The thickness of the lens (measured normal to the lens surface) was measured at 50\(\mu\)m increments in distance from the lens edge along the base curve to the lens centre. The lens thickness data is plotted in figure 8.7a. Note the distance along the base curve has been converted to the polar angle in radians. Figure 8.7b plots a cross-section of the lens geometry showing the base and front curve.

![Graph 8.7a](image)

![Graph 8.7b](image)

**Figure 8.7:** (a) Contact lens thickness data in \(\mu\)m plotted against the polar angle. (b) Contact lens cross-section. Height is measured from the centre of the sphere defining the base curve. Width is the radial horizontal distance from this centre.

This data on the lens dimensions allows us to calculate the final lens volume. The surface area of the back of the lens can of course be calculated exactly from the surface area of the spherical segment. The swelling behaviour of the lens during hydration has been discussed earlier. During hydration the lens volume increases substantially during PG dosing, before decreasing again during DI dos-
8. CHEMICAL TRANSPORT IN THE CONTACT LENS HYDRATION PROCESS

The final lens volume is still larger than the initial lens volume. No data is available on the lens swelling times, but the industry collaborator estimates that the lenses may take 5–10 minutes to reach equilibrium PG concentration, but 20–30 minutes to release from the front curve. Data is available on the linear increase in lens dimensions following PG hydration. Assuming the hydration is at approximately 90°C the linear increase in lens dimensions is 12–13%. Following DI dosing the linear increase in lens dimensions from the original dry lens is about 4%. The volume of the final lens is estimated to be 0.0402 cm³. Applying the linear change in dimensions to the lens thickness data and the length along the base curve (but keeping the spherical radius of the base curve fixed) we can estimate the initial volume of the lens as 0.0359 cm³ and the volume following PG dosing as 0.0510 cm³. The volume increase in the lens following PG dosing is about 42%, while it is about 12% following the DI dosing, both relative to the initial lens volume.

The volume data allows us to get some estimate of the volume of PG in the lens following PG dosing. We assume that the PG occupies the 42% increase in volume. Also as the D3O is now all displaced we also assume that the PG occupies the initial volume occupied by the D3O. We know the lens is 23% D3O by mass. We make the assumption that it is also 23% by volume. Thus we estimate the volume of PG in the lens is approximately 0.0289 cm³. Similarly the final volume of DI in the lenses is estimated as 0.0182 cm³. The surface area of the base curve of the final lens is 2.092 cm². The estimated surface areas of the initial lens and lens following PG dosing are 1.946 cm² and 2.433 cm² respectively. The average (final) lens thickness is 178 µm. The estimation of lens volume, surface area and average thickness should be useful when estimating the mass transfer coefficient in lens extraction models.

Figure 8.6: Lens geometry
8.3 Modelling of chemical transport in the hydration process

The goal in this section is to outline a model which can describe the dynamics of extraction in the hydration process, with a view to analysing the key questions outlined earlier. The models will be based on D3O extraction with PG but if similar kinetics can be shown to apply to the extraction of PG during the DI dosing period, similar models can be used in that case. Before considering more complicated models, we consider some index averaged models to provide some rough estimates of the concentrations in tanks and concentration differences between extraction fluid in the top and bottom of stacks.

8.3.1 Steady state mass balance models for an index time

8.3.1.1 Modelling average tank concentration over an index time

We consider a simple mass balance model to calculate the average concentration in each of the tanks over an index time at steady state. The concentration will vary within an index time. However, provided the inflow mass of D3O in the lenses to the system per index and the inflow volume (or mass) of fresh PG into the system per index is constant and the process variables are fixed, then it is reasonable to assume that the average concentration in each of the tanks will reach a steady value. We will formulate the model in relation to D3O in the mini-stack rig. The generalisation to different numbers of stages and to DI extraction of PG should be clear.

We consider each pair of a stack and a tank as a unit and consider mass flow of D3O in and out of a unit. We are assuming a steady state for each unit so mass flow of D3O in, over an index time, must be equal to mass flow of D3O out, during an index time. Considering stage 1 we have

\[ \text{D3O in lenses in incoming stack + D3O entering in flow from tank 2} \]
\[ = \text{D3O in lenses in exiting stack + D3O leaving in flow from tank 1} \] (8.3.1)

We write this in terms of the mass of D3O per mass of dry lens and the average
concentration (mass per volume) of D3O in the tanks, as follows

\[ f_{01} m_t n_t T_w Q_1 c_{d,2} = f_{12} m_t n_t T_w Q_1 c_{d,1}, \]  

(8.3.2)

where

- \( f_{ij} \) is the average mass fraction of D3O (per mass dry lens) in the lenses leaving stage \( i \) and entering stage \( j = i + 1 \),
- \( m_l \) is the mass of an individual lens,
- \( n_l \) is the number of lenses in a tray,
- \( n_t \) is the number of trays in a stack,
- \( T_w \) is the index time,
- \( Q_1 \) is the average volume flow rate from tank 2 to tank 1 during the index time,
- \( c_{d,i} \) is the average concentration in tank \( i \) during an index time.

We can rearrange this as

\[ c_{d,2} - c_{d,1} = \frac{m_l n_t}{T_w Q_1} (f_{12} - f_{01}). \]  

(8.3.3)

We can relate this to an effective dose (refresh volume of PG in an index divided by number of lenses in a stack) defined as

\[ E_d = \frac{T_w Q_1}{n_l n_t}. \]  

(8.3.4)

Then

\[ c_{d,2} - c_{d,1} = \frac{m_l}{E_d} (f_{12} - f_{01}), \]  

(8.3.5)

For the mini-stack rig, for the mass transfers shown in figure 8.8, we have the following three equations:

\[ c_{d,2} - c_{d,1} = \frac{m_l}{E_d} (f_{12} - f_{01}), \]  

(8.3.6)

\[ c_{d,3} - c_{d,2} = \frac{m_l}{E_d} (f_{23} - f_{12}), \]  

(8.3.7)

\[ c_{in} - c_{d,3} = \frac{m_l}{E_d} (f_{34} - f_{23}). \]  

(8.3.8)
For any process, we should know the concentration of D3O in the incoming PG and the mass fraction of D3O in the incoming lenses. Thus if we measure the mass fractions \( f_{ij} \) we can solve for the average concentrations and vice versa. We can combine these equations to find the mass balance for consecutive stages. Adding the three equations gives

\[
c_{in} - c_{d,1} = \frac{m_l}{E_d} (f_{34} - f_{01}). \tag{8.3.9}
\]

This is the mass balance for the three dosing PG stages, which we can use to estimate the average concentration in tank 1, i.e. the average concentration of D3O in the PG leaving the system. For example, suppose we consider an extraction on the mini-stack rig, with an index time of \( T_w = 900 \) s, a refresh rate \( Q_1 = 11 \text{min}^{-1} \), a mass fraction of 0.23 (230000 ppm) in the entering lenses and a mass fraction of 0.0002 (200 ppm) in the exiting lenses. Let the D3O concentration in the entering PG be 0 kg m\(^{-3}\). The mass of entering lenses is \( m_l = 0.05 \text{g} \) while \( n_l = 64 \) and \( n_t = 30 \). Then the average concentration in tank 1 is 1.4702 kg m\(^{-3}\) or approximately 1470 ppm. For the production line we have 6 PG dosing stages with \( T_w = 450 \) s and a refresh rate \( Q_1 = 41 \text{min}^{-1} \). Assuming that the lenses are cleaned to the same level of 0.0002 (200 ppm) we find that the average concentration in tank 1 is 0.735 kg m\(^{-3}\) or approximately 735 ppm. Here the index time has halved but the refresh rate has increased by a factor of four. Thus the effective dose has doubled leading to a halving of the concentration in
the PG exiting the system.

It should be noted that the mass fraction of D3O that the lenses are cleaned to clearly depends on the system parameters. However provided the final mass fraction is sufficiently small relative to the initial mass fraction than the estimate of average concentration in the PG exiting the first tank should be quite accurate. For example, increasing the final D3O concentration in the lens to 2000 ppm for the production line calculation only reduces the average exiting concentration to 730 ppm in tank 1. Note that the D3O concentrations of PG in the system are inversely proportional to the effective dose. Thus the gain of increasing the effective dose in terms of maximising the concentration gradient between the lenses and the fluid will decrease with increasing effective dose. The most gain should be in the last stage where the gradient is smallest.

8.3.1.2 Modelling average concentration difference in a stack

We can easily expand on this model to estimate the average difference in concentration of D3O in the PG fluid in the top and bottom of the stacks over an index time. The concentration at the top is just equal to the average concentration in the tanks, except in stage 3, where it is equal to the concentration in the incoming PG $c_{in}$. Here we just consider each stack and tank in each stage as a unit and look at mass balance between them. We denote the concentration of D3O in PG fluid exiting stack $i$ by $c_{a,i}$. Thus the 6 balance equations for the ministack rig system take the form

\[ c_{d,1} - c_{d,2} = \frac{Q_1}{Q_1} (c_{a,1} - c_{d,1}) , \]  
\[ c_{a,1} - c_{d,1} = \frac{Q_1 m_l}{Q_1 E_d} (f_{01} - f_{12}) , \]  
\[ c_{d,2} - c_{d,3} = \frac{Q_1}{Q_1} (c_{a,2} - c_{d,2}) , \]  
\[ c_{a,2} - c_{d,2} = \frac{Q_1 m_l}{Q_1 E_d} (f_{12} - f_{23}) , \]  
\[ c_{d,3} = c_{a,3} , \]  
\[ c_{a,3} - c_{in} = \frac{m_l}{E_d} (f_{23} - f_{34}) . \]

Using the June deconstruct data, we can calculate the average tanks concentrations and average stack exiting concentrations for these experiments. The
results for index times of 600 s and 900 s with weir flow rates $Q_1$ of 1.61 min$^{-1}$ and 1.11 min$^{-1}$ are shown in figure 8.9. The flow rate to and from stacks $Q_4$ is 5.1 min$^{-1}$. It is clear that increasing the effective dose will reduce the average tank concentrations as the concentration is inversely proportional to the effective dose. Increasing the flow rate to the stacks $Q_4$, relative to the weir flow rate $Q_1$ will reduce the concentration difference from top to bottom of a stack relative to the tank concentration except in the last stage.

In table 8.1, the concentration ranges in the lenses for each stage during experiments with index times of 600 s and 900 s are compared with the calculated average values in the tanks and the stack exit. Care needs to be taken when comparing these values, which are based on average values and don’t consider volume changes in the lens. However it does appear that the reduction in the concentration gradient due to concentration differences between the top and bottom of stack is certainly less than 1%. It is also clear that, if the incoming PG is contaminated with D3O, the impact of this on the concentration gradient (and thus extraction) will be mostly on in the last stage.
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<table>
<thead>
<tr>
<th>Index Time</th>
<th>900 s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stage</td>
<td>1</td>
</tr>
<tr>
<td>Lens</td>
<td>230000–2974</td>
</tr>
<tr>
<td>Tank</td>
<td>1471</td>
</tr>
<tr>
<td>Stack Exit</td>
<td>1762</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Index Time</th>
<th>600 s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stage</td>
<td>1</td>
</tr>
<tr>
<td>Lens</td>
<td>230000–6261</td>
</tr>
<tr>
<td>Tank</td>
<td>1377</td>
</tr>
<tr>
<td>Stack Exit</td>
<td>1807</td>
</tr>
</tbody>
</table>

**Table 8.1:** Table of D3O concentration ranges in lenses in ppm (data) and calculated average tank and stack exit D3O concentrations in PG fluid in ppm.

### 8.3.2 Time and space dependent models

We will consider some extraction models which can be solved to give D3O concentrations at any given time during the hydration process. It is clear that many variables which influence the process, such as temperature and lens volume, change throughout the extraction time. The extraction rate will likely depend on these changes. However without data on these variables, the nature of the dependence cannot be determined. It is clear that these variables depend on time, so we will discuss them as time-dependent quantities, while recognising that this dependence may be through temperature or volume changes. Similarly, where models are spatially dependent, we will discuss variation of quantities with stack height, while again recognising that this dependence may be the result of a temperature difference. Ideally we would like lens volume and temperature to be explicitly related to time and position and the dependence of, for example, extraction rate on lens volume and temperature to be defined. However this does not seem possible with the current data and knowledge of the process available.

### 8.3.3 Compartment model of chemical transport in the hydration process

The steady state mass balance model discussed previously is useful but somewhat limited. While it captures some fundamental behaviour of the system, it only looks at index averaged concentrations. In addition measurement of either, the
(average) mass fraction of D3O in the lenses after each stage, or the average D3O concentration in the tanks over an index, is needed to fully resolve the model. A more useful model would provide initial conditions for D3O mass fraction in the incoming lenses, the D3O concentration in the PG and describe the dynamics of the extraction from this initial state. One useful way to describe the chemical extraction in the system is to split the process into different compartments in the system which contain D3O. We then model extraction by forming mass balance equations for each of the compartments, to describe the transfers of mass in the system. The number of compartments we choose depends on the scale on which we want to resolve the system. For example, if we believe that all lenses extract at approximately the same rate, we might just describe all the lenses in one stack as one compartment, with uniform concentration. If we believe lenses extract differently based on position, we might assign different compartments to lenses in each tray, or even to each individual lens. Mass distribution within each compartment is often assumed homogeneous (compartment is well-mixed), but it can also have spatial dependence, if required. However, with increasing complexity comes a greater need for experimental data and insight to motivate, parametrise and ultimately validate the model.

We start with a simple compartment model, which we introduce based on D3O extraction in the mini-stack rig. In the mini-stack rig, we have five dosing stages: three PG stages and two DI stages. In terms of D3O extraction, we just consider the first three stages. Within each stage, D3O can be contained in the PG fluid in the tank, the PG fluid in the stack or within the lenses. Thus we have three compartments in each stage. For our initial model, we will assume that D3O distribution in the compartments is homogeneous. This is perhaps a reasonable assumption for the tanks, however it may not be so for the lenses or the fluid in the stacks, where there may be concentration gradients, particularly with stack height. We then need to model transport of D3O between the different compartments within and between different stages in the system. There are two main mechanisms for transport of D3O in the system. First, D3O can be extracted from the lenses into the fluid in the stack in each stage. Secondly, D3O can be transported from compartment to compartment by advection in the PG fluid flows in the system.

We denote properties in each of the compartments as follow: the fluid compartment in the stack in stage $i$ is denoted by the subscript $(\cdot)_{a,i}$, the lenses
compartment in stack \( i \) is denoted by the subscript \((\cdot)b,i\) and the fluid compartment in the tank \( i \) is denoted by the subscript \((\cdot)d,i\). Thus the D3O concentrations in the model are denoted by

- \( c_{a,i}(t) \) is the D3O concentration in the fluid in the stack in stage \( i \), at time \( t \).
- \( c_{b,i}(t) \) is the D3O concentration in the lenses in the stack in stage \( i \), at time \( t \).
- \( c_{d,i}(t) \) is the D3O concentration in the tank in stage \( i \), at time \( t \).

We represent concentrations as mass of D3O per unit volume of the compartment considered. Note that, as the compartments are assumed to be well-mixed, the system variables only depend on one independent variable; the time \( t \). It is clear that the volume of each compartment is not constant throughout the process. The volume of fluid in the stack in any stage is likely to vary with inflow rate. Stacks contain no fluid when they enter initially and may partially empty during the drip time of each index. Similarly, the PG volume in the tank will fluctuate due to partial emptying of the stacks during drip time. The volume of PG in the lens increases from zero initially to some equilibrium level, as the lenses absorb PG and swell. Modelling of volume changes in the fluid in the stack and the fluid in the tanks is not difficult and reasonable approximations should be possible by considering the different flow rates and paths during an index time (although the relationship between volume of fluid in the stack and inflow rate is not well understood). Modelling of the volume of PG in a lens is more difficult as there is no data on which to base a description of this process (other than equilibrium linear swell rates of lenses at different temperatures in PG). As a first approximation, in the absence of experimental insight, we neglect volume changes in compartments and adopt their equilibrium values. We will motivate the model in terms of the flows and transfers that occur during the dosing period of the index time in a general stack in the system. It should be clear however that this model is easily adaptable for different flow paths and flow rates between different compartments. The typical flow paths and flow rates during dosing are indicated in figure 6.4a. The main transfers of D3O in a general stage \( i \) are shown in figure 8.10.
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These transfers can be described by the following differential equations:

\[
V_a \frac{dc_{a,i}}{dt} = Q_4(c_{d,i} - c_{a,i}) + \frac{A_b D_c}{r_b} (c_{b,i} - c_{a,i}), \quad (8.3.16)
\]

\[
V_b \frac{dc_{b,i}}{dt} = -\frac{A_b D_c}{r_b} (c_{b,i} - c_{a,i}), \quad (8.3.17)
\]

\[
V_a \frac{dc_{d,i}}{dt} = Q_1(c_{d,i+1} - c_{d,i}) + Q_4(c_{a,i} - c_{d,i}). \quad (8.3.18)
\]

Initial conditions need to be prescribed. Volume fluxes \(Q_1\) and \(Q_4\) can depend on time if necessary. The mass transfer coefficient \(\frac{A_b D_c}{r_b}\) and in particular the diffusion coefficient of chemical from the lenses \(D_c\), should be fitted from experimental data. The volume of the lenses \(V_b\) is ideally the PG volume in the lenses. The diffusion coefficient can be made a function of time either explicitly from experiment or implicitly by relating it to a defined temperature variation. The diffusion coefficient can also be a function of concentration in the lenses.

For D3O extraction, slight variations of these equations are defined for stages \(i = 1, 2, 3\). The equations can be adapted to include back-flushing and drip time, if deemed necessary. To solve these for a given wash cycle we just need the initial concentrations at the start time in each compartment:
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\[ c_{a,i}(t_{\text{start}}) = c_{a0,i}, \quad c_{b,i}(t_{\text{start}}) = c_{b0,i}, \quad c_{d,i}(t_{\text{start}}) = c_{d0,i}, \quad i = 1, 2, 3. \quad (8.3.19) \]

To solve the equations over a number of cycles for index time \( T_w \) one proceeds as follows:

1. Define initial conditions,

2. Solve the equations up to the index time \( t = T_w \).

3. Define new initial conditions for the next index time: tank concentrations and fluid concentrations in stack \( i \) remain the same but the new initial concentrations of lenses in stack \( i \) is the final concentration of lenses of stack \( i - 1 \) from the previous wash. The lenses in first stack are at initial concentration of incoming lenses.

4. Now solve for the next index time.

5. Repeat process to solve for consecutive index times.

6. System should reach steady state after a number of index times.

8.3.4 Compartment model with stack height

The data shows that lenses at the top of the stack extract more than lenses at the bottom. To allow lenses to extract at different rates at different heights in the stack we can introduce more compartments at different heights. Figure 8.11 show a schematic of the transfers for three compartments with stack height. More generally we can introduce compartments for PG solvent and lenses in every tray in a stack. Thus we would have 30 PG fluid and 30 lens compartments in each stack. If we number the equations from \( j = 1, 2, \ldots, 30 \), the equations in stage \( i \)
take the form:

\[
V_{a1} \frac{dc_{a1,i}}{dt} = Q_1(c_{d,i} - c_{a1,i}) + \frac{A_b D_{c1}}{r_b} (c_{b1,i} - c_{a1,i}),
\]

(8.3.20)

\[
V_{b1} \frac{dc_{b1,i}}{dt} = -\frac{A_b D_{c1}}{r_b} (c_{b1,i} - c_{a1,i}),
\]

(8.3.21)

\[
V_{a2} \frac{dc_{a2,i}}{dt} = Q_1(c_{a1,i} - c_{a2,i}) + \frac{A_b D_{c2}}{r_b} (c_{b2,i} - c_{a2,i}),
\]

(8.3.22)

\[
V_{b2} \frac{dc_{b2,i}}{dt} = -\frac{A_b D_{c2}}{r_b} (c_{b2,i} - c_{a2,i}),
\]

(8.3.23)

\[
\vdots,
\]

\[
V_{aj} \frac{dc_{aj,i}}{dt} = Q_1(c_{a(j-1),i} - c_{aj,i}) + \frac{A_b D_{cj}}{r_b} (c_{bj,i} - c_{aj,i}),
\]

(8.3.24)

\[
V_{bj} \frac{dc_{bj,i}}{dt} = -\frac{A_b D_{cj}}{r_b} (c_{bj,i} - c_{aj,i}),
\]

(8.3.25)

\[
\vdots,
\]

\[
V_d \frac{dc_{d,i}}{dt} = Q_1(c_{d,i+1} - c_{d,i}) + Q_4(c_{a30,i} - c_{d,i}).
\]

(8.3.26)

Again initial conditions need to be defined and the diffusion coefficients \(D_{cj}\) need to be defined, fitted or at least motivated from experiment.

### 8.3.4.1 Compartment model for individual lenses

It is of course possible to have a compartment for each individual lens. This model will also be flexible to account for different extraction rates based on lateral positioning of lenses in a stack. We can also define a distribution of initial D3O concentrations in lenses and/or a distribution of different extraction rates if these factors are deemed significant.

### 8.3.5 Continuous model with stack height

We can approximate the properties of the fluid and lens compartments in a stack by considering them as continua. The simplest such model is to consider properties to be homogeneous in any cross-section and vary with stack height. We define stack height by the coordinate \(z\), where \(z\) varies from zero at the top of stack (fluid entrance), to \(L\) at the stack bottom (fluid exit). D3O concentrations in the PG solvent and lenses are defined to depend on the vertical coordinate and time as shown in the schematic in figure 8.12.
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Figure 8.11: Compartment model with stack height.

Figure 8.12: Continuous model with stack height.
The model equations in this case take the form:

\[
V_a \frac{\partial c_{a,i}}{\partial t} = -LQ_4 \frac{\partial c_{a,i}}{\partial z} + \frac{A_b D_c}{r_b} (c_{b,i} - c_{a,i}),
\]  \hspace{1cm} (8.3.27)

\[
V_b \frac{\partial c_{b,i}}{\partial t} = -\frac{A_b D_c}{r_b} (c_{b,i} - c_{a,i}),
\]  \hspace{1cm} (8.3.28)

\[
V_d \frac{\partial c_{d,i}}{\partial t} = Q_1 (c_{d,i+1} - c_{d,i}) + Q_4 (c_{a,i}(L,t) - c_{d,i}).
\]  \hspace{1cm} (8.3.29)

The diffusion coefficient can be defined as a function of stack height and time. For example, equation (8.2.13) can be adjusted to depend on stack height via the following equation:

\[
D_i = \left(1 - \left(\frac{z}{L}\right)^2 \delta_L\right) \left(D_0 + (D_\infty - D_0)(1 - e^{-kt})\right),
\]  \hspace{1cm} (8.3.30)

where \(\delta_L\) is the fractional drop in the diffusion coefficient from the top to the bottom of the stack. The parameter \(\delta_L\) can be estimated from data on the ministack rig. Note the model assumes constant volume of the lenses. As with all the models presented, if a physical model, or empirical formula for lens volume change can be found then this assumption can be relaxed.

### 8.3.5.1 Continuous model with stack height and width

We can extend the continuous model to include width as an extra spatial dimension and allow properties to vary with lateral position in the stack if necessary. Alternatively, we can assign a compartment to each individual column and allow the diffusion coefficient to depend on the position of the column in the stack as well as the stack height. One way of doing this is to divide columns according to their distance from the centre of the stack. For example, if we use the regions \(p = 0, 1, 2, 3\) shown in figure [8.13](#), we could define the diffusion coefficient

\[
D_i = \left(1 - \left(\frac{z}{L}\right)^2 \left(\delta_L + \frac{p}{3} \delta_w\right)\right) \left(D_0 + (D_\infty - D_0)(1 - e^{-kt})\right),
\]  \hspace{1cm} (8.3.31)
with $\delta_w$ being the fraction drop in the diffusion coefficient from bottom centre position to bottom edge.

### 8.4 Model simulations: Mini-stack rig

A number of the models presented in the previous section, describing D3O extraction in the hydration process, have been implemented in MATLAB®. The main three models fitted are

- D3O model fitted to data: No temperature variation, top-bottom positional variation is only attributed to a reduced concentration gradient.

- D3O model fitted to data: Time-dependent diffusion coefficient, top-bottom positional variation is only attributed to a reduced concentration gradient.

- D3O model fitted to data: Time and position dependent diffusion coefficient, top-bottom positional variation is attributed to reduced concentration gradient and position varying diffusion coefficient.

As the data, indicates a dependence on stack height, each of these models is based on equations $(8.3.27)-(8.3.29)$. The model equations are altered to get the three cases above by changing the form of the diffusion coefficient. A further model which simulates each column in a stack separately is also implemented, but this there is insufficient data to parametrise such a model. No models are implemented for PG extraction with water, as extraction mechanism is not clear from data.

For the model simulations presented here we will assume:

- The volume of PG in a lens is constant and equal to the final volume of PG in the lens. This is estimated in section $(8.2.5)$, from lens geometry and linear swelling data from experiments.

- The lens surface area $A_l$ and diffusion distance $r_l$ are constant and estimated from lens geometry.

- The initial concentration of D3O in the dry lenses is 230000 ppm mass D3O per mass of dry lens.

- The diffusion coefficient can be defined as a function of time and position (e.g. as a proxy for temperature) to fit experimental extraction profiles.
Initially, we consider the model in section 8.3.5 which allows for concentration variation with stack height. We assume that the diffusion coefficient is constant and the initial concentration in the lens corresponds to 230000 ppm of D3O. The diffusion coefficient is chosen to fit the mini-stack rig data shown in figure 8.2. The model is solved for 20 index times until a steady state is reached. As discussed earlier, it is not possible for this model to fit the data with the prescribed initial condition. A comparison between the extraction curve for lenses in the top and the bottom positions during hydration for the model, with diffusion coefficient $D_c = 0.73 \times 10^{-10} \text{m}^2\text{s}^{-1}$, and experimental data is shown in figure 8.14. As the model does not account for the different behaviour during the non-isothermal extraction in the first stage, it is not flexible enough to fit both the initial condition and the data from the isothermal extraction period. To rectify this we need to introduce extra degrees of freedom into the model as discussed earlier.

There are a number of ways of extending the model. We could choose a new lower initial concentration by extrapolating the log-linear fit of the mini-stack rig data. This corresponds to the assumption that a large amount of the D3O
initially present in the lens extracts almost instantaneously, while the remaining D3O extracts with a constant diffusion coefficient. An alternative to this, that was discussed in section 8.2.1.2, is to split the D3O mass into fast and slow extracting groups, each with their own diffusion coefficient. The diffusion coefficient for the fast extracting group can be chosen to deplete its mass over the first stage. Instead here we will define a time dependent diffusion coefficient, which will transition from an initially high diffusion coefficient to one which fits the extraction curve to the data after the first stage of extraction.

### 8.4.2 Model 2: Time dependent diffusion coefficient

Here we adapt model 1, by replacing the constant diffusion coefficient $D_c$ with a time varying diffusion coefficient as defined in equation (8.2.13):

$$D_c = D_0 + (D_\infty - D_0)(1 - e^{-kt}).$$

(8.4.1)

The parameter $D_\infty$ is set to match the extraction rate from the data during the isothermal extraction period. The initial diffusion coefficient is $D_0$ and the parameter $k$, determines the timescale over which the diffusion coefficient drops to $D_\infty$. It is important to note that no data is available to choose $k$ or $D_0$ and that the choice of one depends on the other. Here we will choose $k$ so that $D_0$ drops close to $D_\infty$ over the first index time. The choice of $D_0$ is then made to ensure that the extraction curve goes through the data points in the isothermal period. The wrong choice of the pair $D_0$ and $k$ will lead to the extraction curve being above or below the data points during the isothermal extraction despite having the right extraction rate.

To fit the data from the mini-stack rig, we choose $D_\infty = 4.736 \times 10^{-11} \text{ m}^2 \text{s}^{-1}$. We then choose $k = 1/220 \text{s}^{-1}$ so that $D_0$ decays to $D_\infty$ over a timescale of 220 s. We set $D_0 = 4 \times 10^{-10} \text{ m}^2 \text{s}^{-1}$ to match extraction curve to data. The extraction curves for the lenses in the top and the bottom positions during hydration are plotted against data in figure 8.15. Using a time dependent diffusion coefficient allows us to fit both the data and the initial conditions. The simulations show that the difference in the concentration gradient between the top and the bottom positions in the stack has little influence on the final lens concentration. The final difference is approximately 4 ppm. In order to reproduce the observed differences
8.4 Model simulations: Mini-stack rig

in lens concentration from the top to bottom in the stack we can define the diffusion coefficient to depend on stack height.

8.4.3 Model 3: Time and position dependent diffusion coefficient

In section 8.2.2, it was determined that on average the final D3O concentration in lenses in the bottom of the stack was higher than in those at the top. The industry partner feels this is a result of the temperature difference between the top and the bottom of the stack. There is insufficient data to be certain about this and the experimental set-up does not allow any correlations between extraction rate and temperature to be established. The model in the previous section suggests that the observed differences cannot be solely down to a smaller concentration gradient at the bottom positions in the stack. Thus a temperature dependent extraction remains the most likely cause of the observed differences.

The Stokes-Einstein-Sutherland equation

The Stokes-Einstein-Sutherland equation relates the diffusion coefficient for spherical particles in a fluid to the
temperature and viscosity of the fluid. The diffusion coefficient is given by

\[ D = \frac{k_B T}{6\pi \eta r}, \]  

(8.4.2)

where \( k_B \) and \( r \) are constants and \( T \) and \( \eta \) are the fluid temperature and dynamic viscosity. The equation was derived independently by William Sutherland and Albert Einstein in 1905. It is not possible to use this formula to estimate our diffusion coefficient, but it may be useful to get an idea of how the diffusion coefficient might vary with temperature. Suppose we want to compare the diffusion coefficient for D3O in PG at two different temperatures \( T_1 \) and \( T_2 \) with corresponding viscosities \( \eta_{T_1} \) and \( \eta_{T_2} \). Using equation (8.4.2) we can write

\[ \frac{D_{T_1}}{D_{T_2}} = \frac{\eta_{T_1}}{\eta_{T_2}} \frac{T_2}{T_1}. \]  

(8.4.3)

Using this equation, we can compare the diffusion coefficient for PG at two different temperatures provided we know their viscosities at those temperatures. Thus, if we fit the diffusion coefficient \( D_{88} \) for the top lenses in the mini-stack rig (\( T_2 = 88^\circ C \)), we can estimate how much lower the diffusion coefficient is at the bottom for a temperature of say (\( T_1 = 83^\circ C \)) using the viscosities for PG at these temperatures. The viscosities of PG at various temperatures can be found in ref. [16]. Figure 8.16 shows a comparison of the diffusion coefficients are various temperatures to the diffusion coefficients at 88°C and 96°C. These correspond to the set point temperatures for PG dosing on the mini-stack rig and in the production process respectively. If we assume a steady state temperature drop in the stack of 5°C from top to bottom, then then we see the diffusion coefficient is about 6% lower at the bottom compared to the top for the mini-stack rig. At the higher temperatures of the production process, the drop is more pronounced, as the rate of change of viscosity with temperature is higher. A 5°C drop here results in about a 15% drop in the diffusion coefficient from top to bottom in the stack. This suggests that the difference in final lens concentration based on position will be emphasised at production temperatures. However, as the bottom temperature in the production line is higher than the top temperature in the mini-stack rig, all lenses should be cleaned more efficiently in the production process relative to the mini-stack rig.
8.5 Model simulations: Production line

The previous paragraph gives some justification to the suggestion that extraction may be temperature dependent and thus the diffusion coefficient should be modelled as being temperature dependent. One way of implementing this, would be to extend the models in chapter 7 to model temperature in the fluid in the stack based on height and possibly width, and couple this model with the model of D3O extraction. Instead, given the limited data available, we will let the diffusion coefficient depend on position (as a proxy for temperature) as suggested in section 8.3.5. Thus the diffusion coefficient is set to

$$D_c = \left(1 - \left(\frac{z}{L}\right)\delta_L\right)\left(D_0 + (D_\infty - D_0)(1 - e^{-kt})\right), \quad (8.4.4)$$

where $\delta_L$ is the fractional drop from top to bottom of the stack. Motivated by the discussion above we choose $\delta_L = 0.06$. The resulting extraction curves for the top and bottom positions are shown in figure 8.17.

The positional dependence can be extended further by making the diffusion coefficient dependent on the position of the column in the stack as described by equation (8.3.31) in section 8.3.5.1. This model will be referred to as model 4.

8.5 Model simulations: Production line

We have a number of models available to consider the key questions for chemical extraction for the production line specifications. Given the limited data and the degree of variability in the observed data from lens to lens, it is difficult of fit the models which allow positional variation in extraction at this stage. Nevertheless
we will consider all models here and verify that we arrive at the same conclusions. For model 2, the diffusion coefficient can be fitted to the slowest extracting lens in the stack. The more sophisticated models 3 and 4, can be used to verify the conclusions from model 2, but without improved data to fit the extra degrees of freedom, there is little to be gained from favouring these models over model 2.

Having chosen a model, the second question is what model parameter values we should use for the production line process. The model allows parameters such as the flow rates, no. of stacks in each stage and tank sizes to be easily altered to the production line specifications. The key question is how the extraction rate (via the diffusion coefficient) changes for the production line process given the higher processing temperatures. Unfortunately, as mentioned previously, the correlation between extraction rate and temperature cannot be determined from available experimental data. Thus the fitted diffusion coefficient functions from the mini-stack rig, will be used for the production line simulations. As the temperatures are higher in the production line, this should mean we tend to underestimate the extraction rate and overestimate the concentration in the final lenses.

In the following sections we look at some simulations of D3O extraction on the
production line in the context of the three initial questions posed by the industry partner.

### 8.5.1 Blocked nozzle

From time to time a nozzle in one of the shower-heads in the hydration system may get partially or fully blocked. This means one column of lenses in a stack will miss out on one full dosing stage. On the production line, this means the extraction time for these lenses is cut by 450 s. This may lead to lenses not being cleaned to specification. The blocked nozzle may not be identified for some time, which may lead to a large number of lenses being out of specification. We consider here the effect of a blocked nozzle on the final lens concentration and whether this depends on what stack or column the blocked nozzle is in. We also investigate what final concentration in the lens under normal operating conditions will result in the lens still being within specification if a nozzle is blocked in one stack. We do not consider the effect of multiple blocked nozzles. A blocked nozzle is a rare event, so assuming that the blocking of nozzles in different stages are independent events, the probability of having two blocked nozzles in different stages at the same tray position, at the same time, is extremely low.

Before looking at more model simulations, it is possible to get a quick estimate of the effect of a blocked nozzle. A blocked nozzle means the lenses in question miss one stage of the extraction. Assuming this effect is independent of the stage in question, we can get an estimate of the increase in the final concentration in the lenses by multiplying the final concentration in normal conditions by the factor $e^{bt_w}$. Here $t_w$ is the index time and $b$ is the negative of the slope of the fit to the log of the lens concentration.

Considering either models 2 or 3, we can simulate a blocked nozzle by “switching off” extraction in one stack. This is done by setting the diffusion coefficient in that stack to zero. If the diffusion coefficient is time dependent it is adjusted to account for this, so that the time is the actual extraction time the lens experiences rather than the time since the lens enters the process. Figure 8.18 shows the extraction profile of lenses for different simulations of model 3 at the top position. The curves are labelled by the stage in which the diffusion coefficient is set to zero. The curve marked zero has no blocked nozzle. It can be seen that within the resolution of the graph the increase in final concentration seems to be
independent of the stage in which the nozzle is blocked. However, if we look a little closer at the final concentrations, they do reveal that the stage in which the nozzle is blocked affects the final lens concentration.

**Figure 8.18:** Simulated lens extraction profiles at top positions in stack in the production process. Simulations are labelled by the stage in which the diffusion coefficient was set to zero. Simulation ‘0’ had no blocked nozzles.

Figure [8.19](#) shows the final lens concentrations and the increase in the final lens concentration, based on the stage in which the nozzle is blocked. The final concentrations in both the top and bottom positions are shown. These concentrations are compared to those got with the quick estimate outlined above. Comparing the final concentrations, we can see that the effect of a blocked nozzle is slightly more pronounced on later stages than on earlier stages. For example, the final lens concentrations at the top positions for blocked nozzles in stages 1 and 6 are 135 ppm and 139 ppm respectively. The larger influence of a blocked nozzle later in the process, is due to a bigger impact on the concentration gradient here, relative to the earlier stages. We also note that, the quick estimate (which effectively assumes perfect sink conditions in the extracting fluid) gives quite a good upper bound on the effect of a blocked nozzle. Thus to remain within specifications (i.e. a final D3O concentration less than 200 ppm) the final concentration under normal operating conditions should be less than $200e^{-bt} \approx 84$ ppm.
Finally, in reality a blocked nozzle does not mean extraction is shut off in a full stage but rather in one column in a stack in the stage. This can be simulated using model 4. In this simulation we can exploit symmetry in the stack to just plot the final concentrations in one quarter of the stack (16 columns). A sample plot with $\delta_L = \delta_w = 0.06$ and a blocked nozzle at position $(1, 1)$ (one of four central columns in the stack) in stage 6, is shown in figure 8.20. The final lens concentration here at the bottom centre position is approximately 220 ppm which compares with a final lens concentration from model 3 at the bottom position of 217 ppm for the equivalent simulation. Note the worst case lens in this model would be at the bottom edge of the stack.

### 8.5.2 D3O concentration in incoming PG

PG solvent exiting the hydration system contains a significant concentration of D3O. Estimates in section 8.3.1.1 suggest that this may average at 700–800 ppm. The PG solvent is expensive, both to purchase and dispose of. Given the large volumes of PG used in the process, there is significant potential for cost savings if
the PG solvent can be reused. D3O can be removed from the contaminated PG using a distillation process. However, it is increasing expensive to remove more of the D3O as the concentration gets lower. Thus, an important question is: what level of D3O in the incoming PG will still result in an effective extraction of D3O from the lenses?

In this section we consider the effect on the final lens concentration of increasing the D3O concentration in the incoming PG. Ideally, in order to determine this, the equilibrium D3O concentration in a lens, for a given D3O concentration in the PG solvent, should be determined experimentally. In the absence of this, we can make some very rough estimates, based on volume arguments. We assume that 100 ppm D3O in the PG surrounding the lens would equilibrate with 100 ppm D3O in the PG fluid in the lens. We have estimated earlier that the volume of PG in the lens after hydration is approximately $2.889 \times 10^{-8}$ m$^3$. This corresponds to about 0.0294 g of PG. As the initial lens mass is 0.05 g, 100 ppm in the PG corresponds to approximately 58.8 ppm mass of D3O per mass of dry lens. Assuming this is correct, than 340 ppm represents the absolute upper bound for the concentration in the incoming PG that could clean the lenses to specification. Here, we compare different concentrations of D3O in the incoming PG and compare the results to perfect sink conditions.
Figure 8.21: (a) Extraction curves for lenses in the top position in the stacks for different incoming concentrations in the PG refresh flow. (b) Extraction curves for lenses in the top position in the stacks for different incoming concentrations in the PG refresh flow in stage 6.

Figure 8.21a compares the extraction profiles of lenses at the top position in the stack using model 3 for different concentrations in the incoming flow. We can see from the plot, that the greatest deviation from the extraction rate in the perfect sink conditions is occurring in the final stage. This is because the higher concentration in the extracting fluid does most damage to the concentration gradient in the last stage, when the concentration in the lens is nearing that in the extraction fluid. Figure 8.21b plots the final concentrations in the top positions in the final PG stage. It is apparent from the plot that a linear increase in the concentration of D3O in the incoming PG results in a linear increase in the final concentration of D3O in the lens over the range of concentrations considered. This corresponds to a shift in the final equilibrium lens concentration. This is also apparent if we plot the final lens concentrations. Figure 8.22 shows the final lens concentrations at both the top and bottom positions and the increase in the final lens concentration relative to fresh incoming PG. For the simulations presented here, each 1 ppm rise in the incoming PG concentration results approximately in a 0.588 ppm rise in the final lens concentration. This relationship should be investigated experimentally.

We can also use the models to consider the change in tank concentrations and consequently the reduction in the concentration gradient between the lenses and the extraction solvent. Figure 8.23a shows the tank concentrations during a typical cycle for different concentrations in the incoming PG flow. We can see that
increasing the concentration of D3O in the incoming PG, increases the concentration in all the tanks by roughly the same amount, decreasing the concentration gradient. Figure 8.23 plots the concentration in the PG in the lenses and in the PG in the tanks, on a log-scale. We can see that the increased concentration in the incoming PG, has relatively little impact on the concentration gradient in the earlier stages, but will start to limit extraction in the later stages.

**Incoming PG flow rate (refresh flow rate)** Before concluding our discussion on D3O concentration in the incoming flow, we consider a related question. Here, we investigate the influence of the incoming flow rate of PG ($Q_1$) on the final lens concentration. This choice may be limited by the choice of heater on the production line. In chapter 7, the heater on the pre-heat tank was sized to allow for an incoming flow rate of 81 min$^{-1}$ to two stacks. We will use model 3 and neglect the effect of the resulting increase or decrease in the temperature drop from top to bottom in the final stack due to the changing flow rate. This means we are using the diffusion coefficient from the mini-stack rig with $\delta_T = 0.06$. The incoming PG is not contaminated by D3O. We vary the flow rate from 21 min$^{-1}$ to 121 min$^{-1}$ and also compare the results with perfect sink extraction conditions.
8.5 Model simulations: Production line

Figure 8.23: (a) Tank concentrations (ppm) during a dosing cycle for different D3O concentrations in the incoming PG. (b) Comparison of tank concentrations and lens concentrations (kg m\(^{-3}\)) for different D3O concentrations in the incoming PG.

Figure 8.24: (a) Lens D3O concentration profiles in final stage for different PG inflow rates at the top positions. (b) Final lens D3O concentrations for different inflow rates at the top and bottom positions.

Figure 8.24a shows the levels of D3O in the lenses in the final PG stage. The final concentrations in the lenses for each flow rate are shown in figure 8.24b. It can be seen that increasing the flow rate has diminishing returns in terms of reducing the final lens concentration. Figures 8.25a and 8.25b show the impact on the tank concentrations of changing the inflow rate. It is clear that the incoming PG flow rate at 8 l min\(^{-1}\) is sufficient to maintain a large concentration difference between the solvent and the solute in the lenses. The tank concentrations are proportional to \(\frac{1}{Q_i}\), so increasing the incoming PG flow rate will have minimal and diminishing returns in terms reducing the final lens concentration as the process
is already relatively close to perfect sink conditions. From this point of view, there is an argument for reducing the inflow rate to reduce the amount of PG used. However this may be damaging through increasing the temperature drop from top to bottom in the stacks in the final stage. This may result in a larger concentration difference between the top and bottom lenses. For example for a flow rate of 21 min\(^{-1}\) (11 min\(^{-1}\) to each stack), experiments in chapter 7 suggest the temperature drop may be as high a 15°C. With reference to figure 8.16, this may lead to a drop of 25% in the extraction rate from top to bottom position in the final stage.

![Figure 8.25:](image)

**Figure 8.25:** (a) Tank concentrations for different inflow rates. (b) Tanks concentrations for different inflow rates (log-scale).

### 8.5.3 Optimum stack height

Increasing the stack height in the system allows an increase in the overall throughput of the system. For the current stack height of 30 trays, experimental data shows that lenses in the top positions are cleaned more efficiently than lenses at the bottom of the stack. Simulations suggest that the observed difference in the final lens concentration, cannot be attributed to a reduced concentration gradient lower in the stack. Thus it appears that the reduced extraction rate is related to a temperature drop in the stack from top to bottom. Increasing the stack height will result in a larger temperature drop and consequently an even slower extraction for lenses at the bottom of the stack. This can be counteracted by increasing the solvent flow-rate through the stacks. However this may have cost implications in terms of increased PG use (if refresh rate is increased) and a
8.6 Conclusions

larger heating requirement. Also the relationship between the temperature drop and the solvent flow rate in the stack would need to be determined and of course practical constraints need to be established. For example, the flow rate cannot be increased indefinitely. Determining the optimum height depends on the process constraints and on the relative importance placed by the industry collaborator on increased throughput compared to increased process costs. Experimental data relating the extraction rate from the lenses to temperature is also required. Thus in the absence of well defined criteria and sufficient data we will not proceed further with addressing the optimum stack height in the production line system.

8.5.4 Extraction of PG with DI

No simulations of the extraction of PG with DI will be presented as the extraction mechanism is not evident from the mini-stack rig data. Models identical to those implemented for D3O extraction with PG can be used but fitting the models is impossible given the large variability in the data.

8.6 Conclusions

In this chapter, we have considered the extraction process in the hydration system outlined in chapter 6. Experimental data for D3O concentration in the lenses during extraction with PG can be fitted with log-linear model (which is to be expected in diffusive systems). No data is available for the initial extraction stage, but it is clear that most of the extraction occurs in the first stage. Thus, the average extraction rate must be much higher during this initial phase of hydration. The data shows that the difference in D3O concentration in the final lens between the top and bottom positions in the stacks is significant. Unfortunately, the structure of the experiments does not allow the temperature dependence of extraction to be determined. The experimental data for PG extraction with DI is highly variable and cannot be modelled. Some positional dependence can be identified as the final concentrations in the top positions are, on average, lower than the bottom positions.

Based on the available data, a number of models were developed to simulate the extraction and transport of D3O in the PG dosing stages. Mass balance models averaged over an index time were applied initially to generate some estimates
of the D3O concentrations in the tanks and stacks in the hydration system. In order to more accurately describe extraction, compartment models describing the extraction and transport of D3O during PG dosing were developed. The key element of these models was the description of extraction from an individual lens. The rate of change of concentration in a lens was assumed to be given by

\[ \frac{dc_l}{dt} = -\frac{D_l A_l}{V_l r_l} (c_l - c_{PG}), \]  

(8.6.1)

where \( V_l \) is the volume of solvent (PG) and solute (D3O) in the lens, \( c_l \) is the concentration of D3O in the lens (mass per unit volume), \( c_{PG} \) is the concentration of D3O in the bulk PG fluid (mass per unit volume), \( D_l \) is the diffusion coefficient, \( A_l \) is the external lens surface area exposed to PG solvent and \( r_l \) is measure of the diffusion distance from the lens interior to the bulk fluid. The extraction from the lens can be made dependent on extraction time (time the lens has been exposed to solvent) and position (location in a stack), by specifying a time and position dependent diffusion coefficient. Four main models are used in simulations of the hydration process. All models divide the hydration system into compartments consisting of PG in tanks, PG in transit through stacks and PG in lenses. The evolution of the concentration of D3O in each of these compartments is modelled. The D3O concentration in the tanks is assumed uniform throughout an individual tank (well-mixed), while the concentration in PG in stacks and lenses is allowed to depend on stack height (models 1–3) and stack height and the column position within the stack (model 4). Model 1 assumes a constant diffusion coefficient. Model 2 has a diffusion coefficient which depends on time allowing for a faster initial extraction to match data. Model 3 incorporates a diffusion coefficient which depends on the vertical position in the stack, allowing lenses lower down in the stack to extract slower in order to match experimental data. This positional dependence can be seen as a proxy for the temperature dependence of extraction. Model 4 extends model 3 to include dependence of the diffusion coefficient on distance a lens is from the centre of the stack.

The D3O transport models are fitted to available data from the mini-stack rig. The models are then extrapolated to describe the production line process by changing the process parameters. The diffusion coefficients fitted to the mini-stack rig data are applied directly to the production line process. In reality, extraction should be faster in the production line process as the temperature of
the extracting PG is higher. However, in the absence of data to correlate the extraction rate with temperature, the conservative assumption of an identical extraction rate was made. These models were then used to address the key questions regarding the process:

1. Influence of a blocked nozzle on final D3O concentration in a lens.
   - An estimate providing a reasonable upper bound for the lens concentration, due to one blocked nozzle in any stage, can be got by multiplying the normal final concentration by a factor $e^{bt_w}$, where $t_w = 450$ s is the index time and $b$ is the negative of the slope of the fit to the log of lens concentration.
   - For the lens to be within specification (< 200 ppm), the normal final concentration of the worst lens has to be less than 84 ppm.
   - The effect of a blocked nozzle is slightly more pronounced in later stages in the process than earlier stages.

2. Critical level of D3O concentration in incoming PG which will still result in lenses being cleaned efficiently.
   - The final lens concentration increases approximately linearly with the increase in D3O concentration in the incoming PG, as the equilibrium D3O concentration in the lens is shifted.
   - For the values used here, a 10 ppm increase in incoming D3O concentration in the PG results in a 5.88 ppm increase in the final lens concentration. This result is strongly reliant on the equilibrium level of D3O in a lens for a given D3O level in the PG solvent being established.

3. Optimum stack height to maximise lens throughput but ensure all lenses are cleaned efficiently.
   - From a concentration gradient point of view, the simulations suggest there is no obstacle to even doubling stack height, as this effect is minimal.
• However, an increase in height will lead to an increased temperature difference between stack top and bottom (unless flow rates are increased to compensate). The impact of this on the final lens concentration, cannot be established as the exact influence of temperature on extraction is not known.

4. Similar questions for PG extraction with DI water.

• The extraction mechanism for PG is not evident from the mini-stack rig data and so no model can be fitted without further data or process knowledge.

• Models similar to the D3O extraction models can be used, but fitting is not possible.

Actions based on the conclusions to the key questions discussed here should not, of course, be made independently of each other. For example, if it is decided to use PG with 20 ppm D3O for the refresh flow than the system will be less robust to a blocked nozzle (and maybe not robust at all). Similarly it may be possible to increase the stack height by 50%, while ensuring all lenses are cleaned to specification, but then reuse of PG with 20 ppm D3O may not be possible. The optimal choice of system parameters should be made to minimise the overall cost accounting for relative risks and benefits of the scenarios described above and other possible scenarios. This is a decision for the industry collaborator and will not be discussed further here.
In this thesis, two independent problems proposed by collaborators from industry were considered. The first problem involved the derivation, from first principles, of a model of the physics of coffee extraction from static coffee bed. The aim of this project was to develop an experimentally validated model of coffee extraction, which has up to this point been missing from the literature. The second problem involved modelling heat and mass transport in a section of a soft contact lens manufacturing process, known as the hydration process. The aims of this project were to determine the size of heating units required in the system and explore the optimal system parameters to ensure the system operates efficiently while minimising the costs incurred. On the surface, the two problems seem quite different, but in fact both situations fall under the general area of heat and mass transport in dispersed flows. Both problems involve the flow of a liquid phase over a solid phase with the aim of leaching soluble content from the solid. The approaches to both problems differ somewhat. In the case of the coffee bed we begin with microscopic mass balance equations and model mass transfer mechanisms on this scale. The microscopic balance equations are averaged over representative elementary volumes in order to derive the macroscale equations. This procedure allows the nature of the macroscale processes to be determined in terms of the microscale properties of the bed. For the hydration system, the focus is on writing down macroscopic balances for mass and energy in the system and using available data to fit the lumped parameters in the model. Both problems
9. CONCLUSIONS

were modelled using a blend of analytical and numerical methods in order to gain insight into the important underlying processes.

9.1 Mathematical modelling of the coffee brewing process

The first part of the thesis, in chapters 2-5, focuses on the development and analysis of a model of flow and extraction in coffee bed during brewing. The study was initiated following on from the presentation of a number of interesting questions regarding the drip filter brewing system, by Philips Research Scientist Freek Suijver, at a study group with industry in the University of Limerick in 2012 [10]. The project aims to address a deficit in the literature which is lacking in an experimentally motivated and validated model of the physics of extraction from a coffee bed during coffee brewing. The model presented here, describes extraction from a static, saturated, doubly porous granular bed. The model is derived from first principles starting with microscopic point balance equations in the different phases in the bed. The bed is divided into a high permeability domain (h-phase), consisting of the pores between the grains, and a low permeability domain (l-phase), consisting of the grains themselves. The granular domain is further divided into void space (v-phase) and granular solids (s-phase). The solid matrix is later characterised depending on whether it is soluble or insoluble and based on its proximity to the grain surfaces. The microscopic point balance equations are averaged, using a volume averaging procedure, to arrive at macroscopic balance equations for coffee solution and coffee solubles in each of the phases. At the macroscale, the phases are represented by overlapping continua. Mass transfers between the phases now appear as source and sink terms in the macroscale balance equations. These terms are defined in terms of the microscale properties of the bed through the averaging procedure.

While the work is motivated by the drip filter brewing system, the model is applicable to any brewing system which consists of a saturated granular bed. The model derivation is open to a number of extension to broaden its applicability to a large set of brewing techniques. The static bed assumption can be relaxed which requires a more sophisticated momentum balance equation than Darcy’s law which has been assumed here. This may be necessary, for example, to model
extraction from a drip filter machine fed by a single jet of hot water which agitates the granular bed. A further extension to consider unsaturated flow during the initial water infiltration is explored in chapter 5. Progress here, is dependent on the determination of the hydraulic properties of the bed. Within the constraints of the current model, its application to two experiments was considered. The model was parametrised for two different coffee grinds, whose grind size distributions were known. Numerical simulations showed that the model could quantitatively reproduce the extraction profiles in the case of a well-mixed dilute suspension of coffee grains and in the case of flow through a packed cylindrical coffee bed. Some microscale parameters could not be measured so fitting parameters were used for the mass transfer coefficients in the system.

9.1.1 Coffee extraction in a well mixed system

In chapter 3, the coffee extraction model is specialised to the case of the well-mixed dilute suspension of coffee grains. Extraction in this well mixed system, can be described by a set of ordinary differential equations. This allows analysis of the extraction kinetics from the coffee grains, independent of transport processes associated with flow through packed coffee beds. Coffee extraction for an individual grain is controlled by two processes: a rapid dissolution of coffee from the grain surfaces in conjunction with a much slower diffusion of coffee through the tortuous intragranular pore network to the grain surfaces. Utilising a small parameter, resulting from the ratio of these two timescales, we constructed asymptotic solutions using the method of matched asymptotic expansions. The asymptotic solutions were compared with numerical solutions and data from coffee extraction experiments. The asymptotic solutions depend on a small number of dimensionless parameters, so the solutions facilitate quick investigation of the influence of various process parameters on the coffee extraction curves.

9.1.2 Coffee extraction from a packed coffee bed

In chapter 4, the coffee extraction model is specialised and analysed in the case of flow through a packed cylindrical bed under the influence of a mechanically imposed pressure gradient. The pressure induces some compression of the granular bed, so the intergranular porosity in fitted using the Kozeny-Carman equation. Asymptotic solutions of the model describing extraction from a packed coffee bed
are developed. These solutions can explicitly relate coffee concentration to the process parameters. For an individual coffee grain, extraction is controlled by a rapid dissolution of coffee from the surface of the grain, in conjunction with a slower diffusion of coffee through the intragranular pore network to the grain surface. Extraction of coffee from the bed, also depends on the speed of advection of coffee from the bed. The small parameter resulting from the ratio of the advection timescale to the grain diffusion timescale was used to construct asymptotic solutions, using the method of matched asymptotic expansions. The solutions in the case of the fine and coarse grinds considered, differ due to a different assumed concentrations following the filling stage. The fine grind has a smaller pore space and much larger specific surface area for extraction. Thus it is assumed that the coffee solution in the bed is at coffee solubility following the initial infiltration. For the coarse grind, the pore space is larger and the specific surface area for extraction is much smaller. It is assumed that the concentration varies linearly from zero at the filter entrance to the initial exiting concentration at the filter exit. The asymptotic solutions were compared to numerical solutions and data from coffee extraction experiments. Again, the asymptotic solutions depend on a small number of dimensionless parameters and so are useful to quickly fit extraction curves and investigate the influence of various process parameters on the extraction.

9.1.3 Infiltration into a dry coffee bed

In chapter 5, the problem of modelling unsaturated flow, during the filling of an initially dry coffee bed, was considered. The various physical processes occurring during infiltration, were outlined and discussed. Some empirical and physical models for liquid infiltration into a porous medium, were considered. A one-dimensional, moving boundary model of infiltration, based on the well established Green-Ampt model, was proposed to describe pressure driven infiltration into a packed bed. The model divides the coffee bed into saturated and dry regions, separated by a moving boundary that propagates into the bed. This model was coupled with coffee extraction equations, in the saturated region, to describe extraction during the infiltration stage. The model was non-dimensionalised, and some exact and asymptotic solutions to the infiltration problem, were presented.
Finally, the model was solved numerically to investigate coffee concentration profiles following completion of the infiltration stage. These profiles were compared with those that had been assumed in earlier chapters for the coarse and fine grinds used. There is scope for some further work at the coffee grain scale, where water infiltration into coffee grains is complicated by evacuation carbon dioxide trapped in the grains’ cellular structures.

9.2 Mathematical modelling of the contact lens hydration process

The second part of the thesis, described in chapters 6–8, involved mathematical modelling of the hydration section of the contact lens process. Hydration involves the removal of undesirable chemicals from the lenses which were used as process aids. In the hydration process considered here, the chemical for removal is called 3,7-dimethyl-3-octanol (D3O). This is removed by washing the lenses in a number of successive stages with propylene glycol (PG) at a temperature of about 96°C. Following this, the lenses are washed with deionised water (DI) at a temperature of 35°C to 55°C. Exiting from the process, lenses have been hydrated with water and detached from their moulds. The hydration process considered in this work has the following characteristics

- Contact lenses, in their front curves, are placed in trays of 64 and stacked in stacks 30 high.
- These stacks pass through a number of PG and DI dosing stations.
- At each station, a shower with 64 nozzles delivers fluid to the stack.
- Each stack has its own heater to ensure fluid reaches set temperature during dosing.
- Fluid cascades down through the stack and washes (hydrates) the lenses.

There were two key objectives of the study of the hydration process. The first was to establish the required heater size for each heating unit on the designed production line heating system. The second was to investigate the influence of changing key system parameters, such as the stack heights and inflow rate of the hydration fluids, on the efficiency of the process in cleaning the lenses.
9. CONCLUSIONS

9.2.1 Heat transport in the hydration process

A number of macroscopic energy balance models were used to describe heat loss and transfers within the hydration system. Output from these models can be used to estimate heater demand in the system, thus providing an estimate of the required heater sizes. One constraint is that the industrial partner would like heating units restricted to just two distinct sizes. Parameters in the models were fitted using available data from a scaled down version of the production line system and material properties. Where data was insufficient to be certain of model parameters, or simplifying assumptions had to be made, care was taken to ensure that results would overestimate rather than underestimate the required heater wattage. The models were implemented in MATLAB\textsuperscript{®}. Heater action was modelling using two techniques. In the first idealised implementation heaters were assumed to deliver the exact wattage required to meet maintain their outlet temperatures at the given set point. The second more realistic approach, was to model heater control by implementing a proportional-integral (PI) controller, which attempts to keep the heater outlet temperature at set point. Some consideration was given to PI controller problems observed in experiments.

The production line hydration system consists of 6 PG stages, 4 DI stages and one stage for disassembling the stacks called the destack stage. Once the models have been parametrised on the experimental rig, they are applied to the production system. Output from the models suggest the following recommendations:

- 9 kW heaters should be sufficient in stages 2–5 and 7–9.

- Tanks 6, which preheats PG at a flow rate of 8 l min\textsuperscript{−1} from 60°C to 96°C, will require an 18 kW heater. It is important to note that if there is any significant increase in the incoming flow rate or decrease in the incoming PG temperature the heater may not be sufficient.

- In order to ensure that the outlet temperature in stage one can be maintained within the stated tolerance of \( \pm 2^\circ\text{C} \), it is recommended that an 18 kW heater be fitted to stage one.

9.2.2 Chemical transport in the hydration process

The primary function of the hydration system is to leach unwanted D3O from the lenses. The industrial partner would like a system which efficiently achieves
this goal, while being robust to common failure modes and minimising the costs incurred. One rare, but damaging, failure mode is when a dosing nozzle in one of the stages becomes fully or partially blocked. This results in a reduced extraction time and, if the problem isn’t picked up immediately, it may result in a large quantity of defective lenses which have to be disposed of. A major cost in the hydration process, is the cost of purchasing and disposing of the PG solvent using. From this viewpoint, it is desirable to identify the amount of PG which has to be delivered to the system in order to maintain an efficient extraction. PG exiting the system has a high concentration of D3O. This can be removed by successively distilling the PG, at an increasing cost to attain a higher purity. Thus, an important question is investigate how clean the PG coming into the system needs to be (keeping other parameters fixed) to efficiently clean the lenses. This ability to reuse PG, may lead to a significant cost saving. Finally, it is desirable to maximise the number of lenses that can be processed by the system per unit time. One way of doing this is to increase the stack height. The question is whether this has any negative impact on the system operation. Similar questions can be asked of the extraction of PG with DI, although in terms of cost they are of less importance, as the costs associated with DI are significantly less than those of PG.

In order to address these questions, a number of mass balance models were developed and fitted to available data for D3O extraction with PG. Due to insufficient data, the extraction of PG with DI was not considered. The extraction of D3O from the lenses was considered as a diffusive process. The key element of the models was the diffusion coefficient which was fitted from available data. This varied from a simple constant, to a time and position dependent function. The temperature of the extracting fluid was not explicitly used in the models, but temperature dependence of extraction was incorporated by defining the diffusion coefficient as a function of stack position. The diffusion coefficients (functions) are then used in models for the production line process. Flow rates, index time, flow paths, tanks sizes etc. are adjusted for production line process but the diffusion coefficient is not adjusted for increased temperature. This is due to the fact that, the nature of the available experiments did not allow the temperature dependence of extraction to be determined. The findings on the key questions are as follows:

- Influence of a blocked nozzle on final D3O concentration in lens.
9. CONCLUSIONS

- An estimate providing a reasonable upper bound for the lens concentration, due to one blocked nozzle, can be got by multiplying the normal final concentration by a factor $e^{bt_w}$, where $t_w = 450\text{ s}$ is the index time and $b$ is the negative of the slope of the fit to the log of lens concentration.

- For the lens to be within specification ($< 200\text{ ppm}$) the normal final concentration of the worst lens has to be $< 84\text{ ppm}$.

- The effect of a blocked nozzle is slightly more pronounced on later stacks than earlier stacks.

- Critical level of D3O concentration in incoming PG which will still result in lenses being cleaned efficiently.
  
  - The final lens concentration increases approximately linearly with the increase in D3O in the incoming PG as the equilibrium D3O value in the lens is shifted.
  
  - For the values used here, a 10ppm increase in incoming D3O concentration in the PG results in a 5.88ppm increase in the final lens concentration. **NB:** This relies strongly on the equilibrium level of D3O in a lens for a given D3O level in the PG solvent being established.

- Optimum stack height to maximise throughput but ensure all lenses are cleaned efficiently.
  
  - From a concentration gradient point of view, simulations suggest there is no obstacle to even doubling stack height as the effect is minimal.
  
  - However, an increase in height will lead to an increased temperature difference between stack top and bottom (unless flow rates are increased to compensate). The result of this cannot be identified as the exact influence of temperature on extraction is not known.

- Similar questions for PG extraction with DI water.
  
  - The extraction mechanism for PG is not evident from the mini-stack rig data and so no model can be fitted without further data or advice from Vistakon.
  
  - Models similar to the D3O extraction models can be used but fitting is not possible.


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