EPSRC

Engineering and Physical Sciences Research Council

InFoMM

Industrially Focused Mathematical Modelling

EPSRC Centre for Doctoral Training in Industrially Focused Mathematical Modelling

Multiphase Modelling of Coffee Bean Roasting

UNIVERSITY OF OXFORD

Nabil Fadai

Jacobs Douwe Egberts

Table of **Contents**

1. Introduction

As one of the most valuable commodities in the world, it is no surprise that the coffee industry is worth more than $100 billion worldwide. Despite this, there has been a significant lack of fundamental research into coffee roasting. Most of the literature on the roasting of coffee beans only present experimental data.

A coffee bean can be described as a porous structure consisting of cellulose, arabinogalactans, lignin, oils, and other organic compounds. Within this porous structure, there are biological cells containing aromatic compounds, water, and various gases. The water and gas components co-exist within the cells, and the aromatic compounds will develop and be released into the coffee bean itself as it is roasted.

The roasting process for coffee beans can be summarised as follows. Freshly harvested coffee beans ("green beans") are first dried before roasting. They are then placed into a drum roaster, where these beans are roasted mainly by contact with a hot air inlet, or into a fluidised bed roaster, where hot air is blown onto coffee beans and are roasted by convection. During this roasting process, the coffee beans change colour from green to a dark brown, and the main coffee aroma compounds are developed. Additionally, the coffee beans will increase in size, as well as lose most of their moisture content. Finally, to stop the roasting process, the beans are transferred to a separate chamber, where they are rapidly cooled to room temperature either with air or liquid water.

A coffee bean is a porous structure which mostly contains water, carbon dioxide, and aromatic compounds.

During the roasting process, the bean's porosity increases, due to the production of CO_2 gas, and because the porous structure is used up in chemical reactions. At the same time, the water within the cells evaporates and becomes water vapour. In consequence, this causes the cells to expand due to increasing gas pressures, and CO_2 gas from the cellulose structure will mix with the water vapour produced in the cells. This expansion also causes the nano-porous walls of the cells to allow more of the gas out of the bean in order to regain equilibrium pressure. These "nano-pores" exist among the cellulose and other organic compounds, and aid in gas transport between cells as well as to the surface of the bean. In Figure 1, we see a typical coffee bean's porous structure after roasting. We can clearly see the pores between the cellulose wall structures in this scanning electron microscope (SEM) image. Before roasting, these pores would contain more liquid water, which are shown as "spots" on the wall structure of the bean. In Figure 2, we see how the bean's porous structure changes during roasting. Due to evaporation and swelling, we can see that a roasted bean's pores are larger and mostly filled with gas.

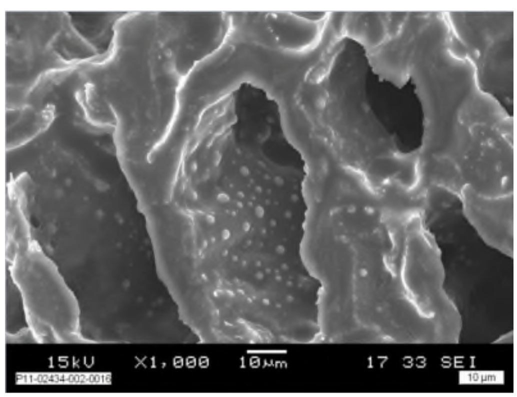

Figure 1: SEM image of the interior of a typical coffee bean after 40 seconds of roasting. Image courtesy of JDE.

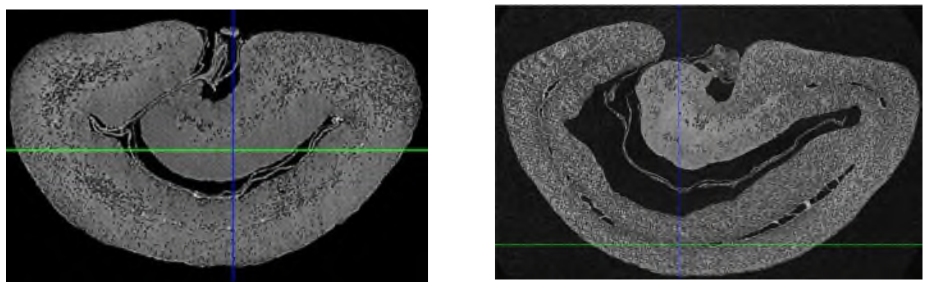

Figure 2: SEM images of a cross-section of a typical coffee bean before roasting (left) and after roasting (right). Image courtesy of JDE.

2. The Multiphase Model

The Multiphase Model is derived from mass and energy conservation equations while also including multiphase flow.

We first derive a coffee bean roasting model using mass and energy conservation laws, and take into account spatial and temporal variation, along with gas and liquid flow. The main results of this modelling are discussed in greater detail in [1]. Firstly, we assume that the cellulose walls degrade as the bean is roasting and produce CO_2, and that the liquid water evaporates. Our model comprises of four coupled conservation of mass equations for the volume fractions of solid coffee, liquid water, water vapour, and CO_2 gas. Additionally, we include an energy conservation equation, where we assume that the dominant heat transport mechanism within the bean is by conduction in all three phases. We note that the main losses of energy occur due to evaporation. Finally, on the surface of the bean, we assume that heat is added to the bean in the roasting chamber by convection.

The dependent variables in the Multiphase Model are the water saturation, water vapour pressure, and temperature.

A visual representation of all of the processes described above is shown in Figure 3. The grey arrows represent CO_2 transport, the light blue arrows represent water vapour transport, the dark blue arrows show liquid water transport, and the red arrows represent heat.

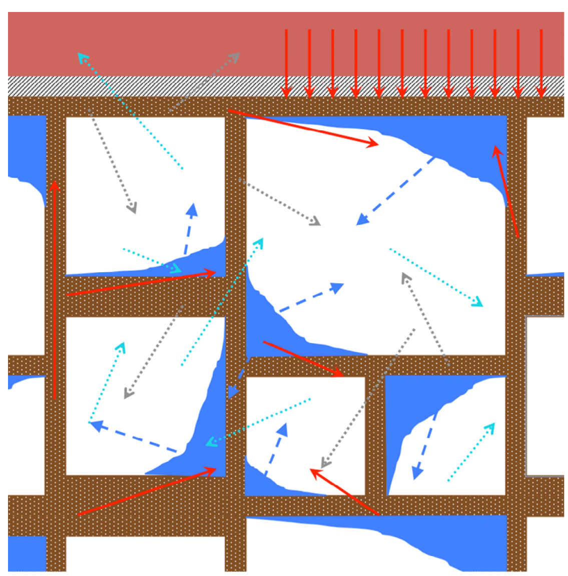

Figure 3: Schematic representation of the Multiphase Model with all transport processes and boundary conditions shown.

While our preliminary model gives us a strong description of processes relevant to the roasting of coffee beans, some parameter values are not found in the literature, making it hard to properly analyse the model. In consequence, we are motivated to simplify this model to gain a preliminary understanding of its equations (denoted as the Multiphase Model). We took parameter values from the literature when possible, and consulted with JDE on appropriate values when they were not readily available.

The Multiphase Model predicts a "drying front" that propagates through to the centre of the bean.

We solved the Multiphase Model numerically, and present the results for the saturation, vapour pressure, and temperature in Figure 4. We see that the liquid water saturation can be divided into two distinct regions in space in time. The first region is where the liquid water saturation has remained at its initial moisture content (red region). The second region, shown in blue, is where the bean has nearly zero moisture content. Additionally, we can see a "drying front" that propagates through towards the centre of the bean, which dries the bean and transitions from the moist region to the dry region. We also note that that the temperature in the coffee bean behaves nearly uniformly in space, as the thermal diffusive timescale of the model is significantly smaller than the vapour diffusive timescale.

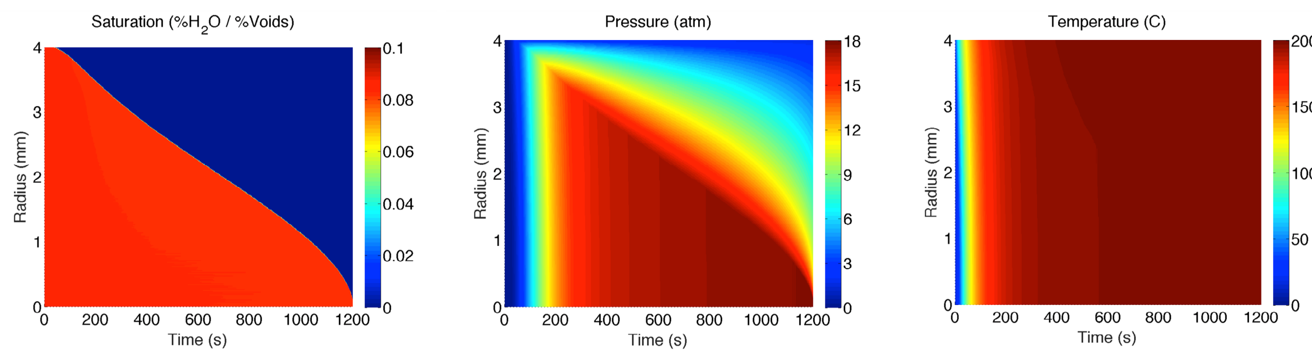

Figure 4: Solutions of the Multiphase Model for 1200 seconds of roasting at 200°C.

3. Comparison of Mathematical Models

A significant difference between the results of Fabbri et al.'s model [2] and the Multiphase Model is how the drying front propagates through the coffee bean. Indeed, while both models predict a drying front that moves to the centre of the bean, the moisture content remaining after the drying front varies significantly. In [2], the authors found that the moisture in the bean slowly decreases after the drying front has reached the centre of the coffee bean, and that the moisture throughout the bean is approximately spatially uniform. In contrast, in the Multiphase Model, the coffee bean is distinctly divided into a moist region and a dry region. Additionally, the drying front in the Multiphase Model moves more slowly than the model in [2]. A comparison of these two models is shown in Figure 5. While both models have been fit to display very similar average moisture concentrations in time (Figure 6), the local behaviour of the bean's moisture content is very different. Given that numerous chemical reactions in the roasting bean depend on the local, rather than average, moisture content, this difference could have important consequences for understanding roasting. For instance, if one chemical reaction requires the local environment to have less than 5% moisture content, the region and time that this could happen in the model presented in [2] is entirely different from the region predicted by the Multiphase Model. In consequence, having a different localized model for the moisture concentration inside a coffee bean can significantly vary the predictions of other chemical reactions that can occur in a bean.

While the model in [2] and the Multiphase Model can both be fit to match the average moisture concentration seen in experimental data, the local moisture concentration differs greatly between the two models.

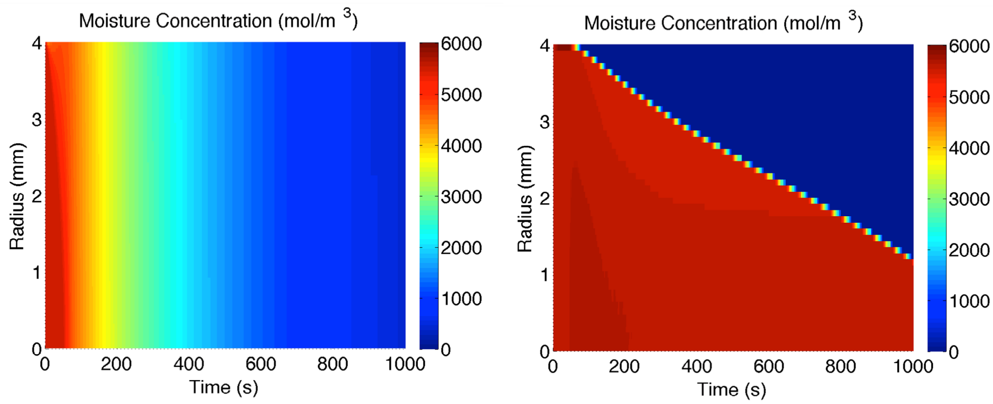

Figure 5: Comparison of the local moisture concentration for 1000 seconds of roasting at 200°C. The model motivated by Fabbri et al. [2] is shown on the left, and the Multiphase Model is shown on the right.

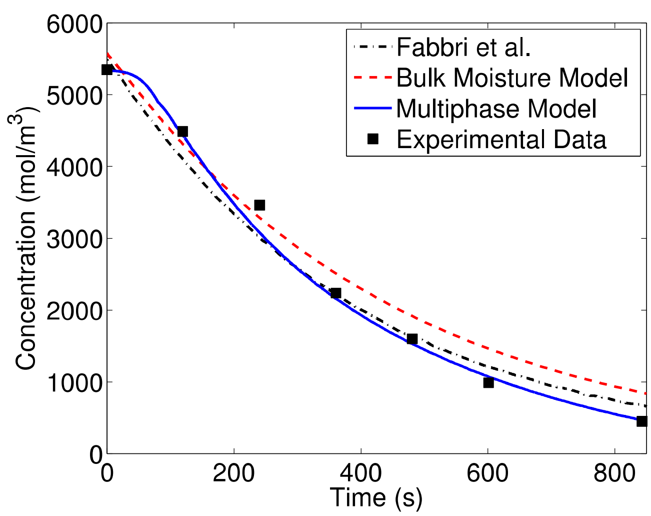

Figure 6: Comparison of the average moisture concentration for 850 seconds of roasting at 200°C. Experimental data is reproduced from [2], the Bulk Moisture Model is based on the model described in [2], and the Multiphase Model is described in Section 2 and in [1].

4. Extensions of the Multiphase Model

Naturally, this preliminary Multiphase Model requires further exploration in various areas. In [3], we examine the Multiphase Model in greater mathematical detail via asymptotic analysis. Specifically, numerical solutions of the Multiphase Model indicate that a “drying front” divides the coffee bean into a moist and dry region, despite the drying front never being prescribed by the model. Using asymptotic analysis, we are able to determine not only the approximate solutions of temperature, water content, and vapour pressure within the roasting coffee bean, but also an approximate form of the observed drying front that agrees well with the numerical solutions (Figure 7).

In [4], we extend the Multiphase Model to incorporate general chemical reaction groups observed in the roasting process (denoted as the Sugar Pathway Model). Additionally, we consider more general geometries and evaporation rates to allow for further agreement between the extended model and new experimental data. While there are several parameters associated with the sugar chemical pathways that are not available in the literature, we note that these unknown parameters are not sensitive to small changes in their values. Hence, the Sugar Pathway Model provides a reasonable qualitative understanding of how to model key chemical reactions that occur in the coffee bean, as well as how to model coffee bean chunks differently to whole coffee beans (Figure 8).

Asymptotic analysis allows us to simplify the Multiphase Model while preserving the salient features of the drying process.

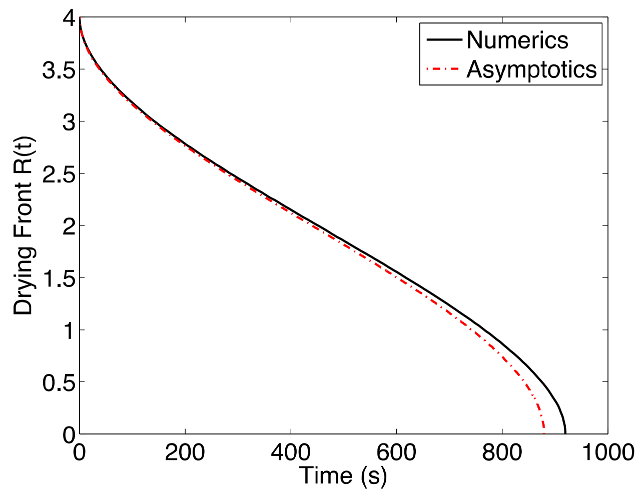

Figure 7: Comparison of the drying front determined from asymptotic analysis, shown in dash-dot red, against the numerical solution of the Multiphase Model, shown in black, in an isothermal setting.

The additional evaporation processes and the incorporation of various geometries in the Sugar Pathway Model allow for the moisture loss to be accurately modelled for coffee bean chunks as well as whole coffee beans.

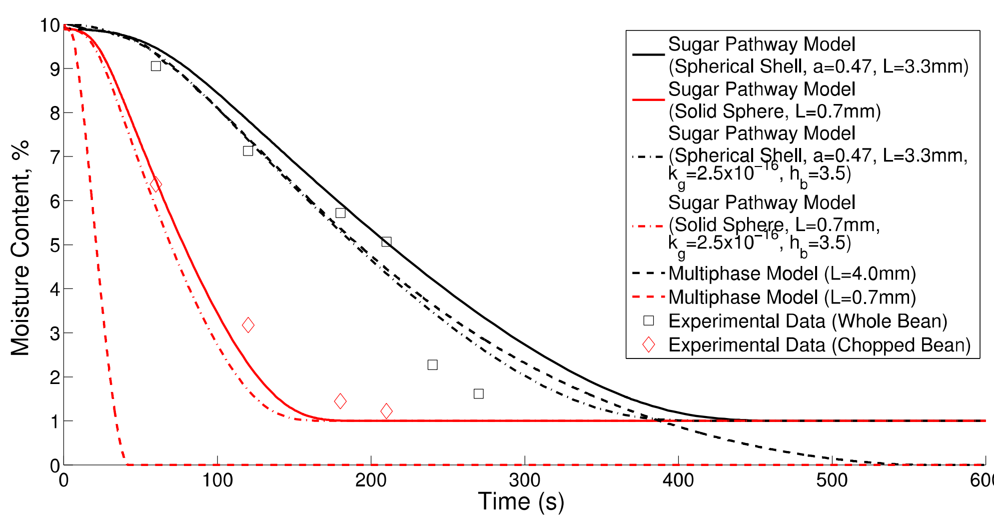

Figure 8: Comparison of the average moisture content in a bean chunk versus a whole bean during a 230°C roast. The solid and dot-dashed lines correspond to the average moisture loss determined by the Sugar Pathway Model described in [4]. The dashed lines correspond to the average moisture loss determined by the Multiphase Model presented in [1], and the markers correspond to experimental data performed at JDE.

Finally, we included elements of solid mechanics in these aforementioned multiphase models. Specifically, we examined how the cellulose structure of the coffee bean changes from a rigid, elastic structure to a viscoelastic material upon exceeding a critical glass transition temperature. This transition temperature depends on the moisture content of the bean and is predicted to first occur in the interior of the bean rather than at the surface. By modelling the cellulose structure as a poroviscoelastic material, we observe that, due to the dramatic change of viscosities at the glass transition temperature, a large build-up of material stress occurs between the onset of the glass transition and when the glass transition occurs at the surface of the bean (Figure 9). This build-up of material stress can be linked to macro-scale deformations and fracturing that occur in the roasting process.

By modelling the cellulose matrix as a temperature-dependent poroviscoelastic material, we can predict macroscale deformations that are due to build-up of internal material stress.

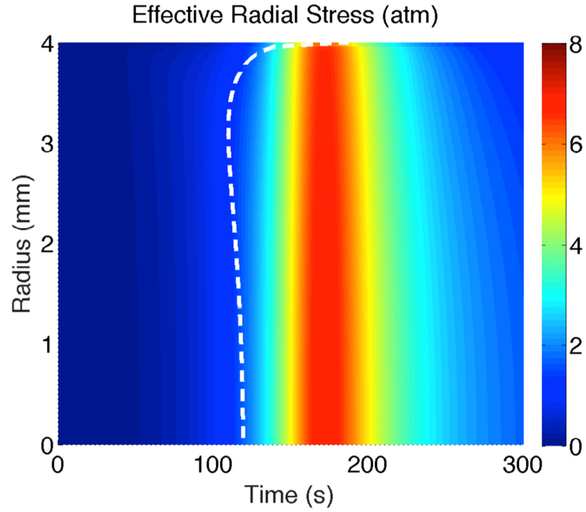

Figure 9: The effective radial stress in the solid cellulose material, predicted using temperature-dependent poroviscoelastic constitutive equations. A large build-up of stress is observed when the glass transition temperature (white dashed curve) approaches the surface of the bean.

5. Conclusions

We have derived various multiphase mathematical models to describe the roasting of a single coffee bean. By simplifying preliminary models (denoted as the Multiphase Model) and fitting parameter values to experimental data, we were able to produce results similar to the experimental data presented in Fabbri et al. [2]. However, the model in [2] involved average moisture concentrations rather than local moisture concentration. In consequence, the Multiphase Model provides better insight into the local behaviour of a coffee bean's moisture concentration. Since coffee drying and coffee roasting rely on different mechanisms to evaporate water, and the model in [2] was tailored to drying rather than roasting, we conclude that the Multiphase Model is better suited to understanding the roasting of coffee beans. Additionally, the presence of a "drying front" that propagates towards the centre of the coffee bean is a key feature of the Multiphase Model. Using asymptotic analysis, we are able to determine an approximate form of this drying front, along with the leading-order dynamics of the water saturation and vapour pressure. Finally, various extensions to the Multiphase Model were considered to capture further qualitiative features observed in the roasting process, including simplified sugar chemical pathways, more physically realistic evaporation rates, and solid deformations within a coffee bean.

Potential Impact

John Melrose of Jacobs Dowe Egberts commented: *"Roasting of coffee beans is the operation in which essentially all the aroma molecules are generated; chemistry which is foundational to the experience of a good cup of coffee. A deeper understanding of the physical and chemical changes that happen during this roasting process can enable more efficient production of high-quality coffee, both at small- and industrial-scale. Dr Nabil Fadai's simulations and analytical work on roasting of a single bean have pointed the way to some important simplifications in our understanding of the heat and water transport through the complex coffee microstructure, and provided a first suggestion for the physical mechanism underlying the "first crack" phenomenon. In artisanal roasting, this acoustic signal is an important control point for ending the roast. Nabil's work represents a significant step forward in a larger programme of modelling the entire roasting process, which we continue to build upon. In addition, Nabil has isolated a boundary-layer problem, within the larger context of the roasting equations, and was able to construct an analytic solution (in a certain asymptotic regime), which was recently published in the SIAM Journal of Applied Mathematics. Fellow researchers in the food industry will appreciate that non-trivial analytic solutions are rather rare in systems as complex as foods, and it is inspiring to see one prised out of a realistic system of PDEs. Such advances help raise the profile of the food industries (the largest manufacturing sector in the UK) as a source of exciting and unsolved technical challenges."*

References

1. N. T. Fadai, J. Melrose, C. P. Please, A. Schulman, R. A. Van Gorder, *A Heat and Mass Transfer Study of Coffee Bean Roasting.* International Journal of Heat and Mass Transfer 104 (2017), pp. 787-799. http://www.sciencedirect.com/science/article/pii/S0017931016311814

2. A. Fabbri, C. Cevoli, L. Alessandrini, S. Romani, *Numerical modelling of heat and mass transfer during coffee roasting process.* Journal of Food Engineering 105 (2011), pp. 264-269.

3. N. T. Fadai, C. P. Please, R. A. Van Gorder, *Asymptotic Analysis of a Multiphase Drying Model Motivated by Coffee Bean Roasting.* SIAM Journal on Applied Mathematics 78 (2018), pp. 418-436. https://epubs.siam.org/doi/abs/10.1137/16M1095500

4. N. T. Fadai, Z. Akram, J. Melrose, F. Guilmineau, C. P. Please, R. A. Van Gorder, *The Influence of Distributed Chemical Reaction Groups in a Multiphase Coffee Bean Roasting Model.* IMA Journal of Applied Mathematics (2018). https://academic.oup.com/imamat/advance-article/doi/10.1093/imamat/hxy023/5021697