EPSRC Centre for Doctoral Training in Industrially Focused Mathematical Modelling

The Roasting of a Single Coffee Bean

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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 has 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.

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

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 either into a drum roaster, where they are roasted through contact with a hot air inlet, or 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 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 using either air or water.

During the roasting process, the bean's porosity increases, due to (i) the production of CO_2 gas, and (ii) the porous structure being used up during 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. We see that, in the bean prior to roasting, the pores are small and largely filled with water. Due to evaporation and swelling, we can see that a roasted bean's pores are larger and mostly filled with gas.

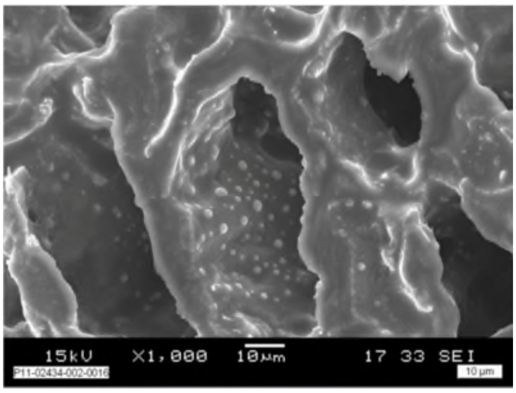

Figure 1: SEM image of the interior of a typical coffee bean after 40 seconds of roasting. Image courtesy of Mondelez International.

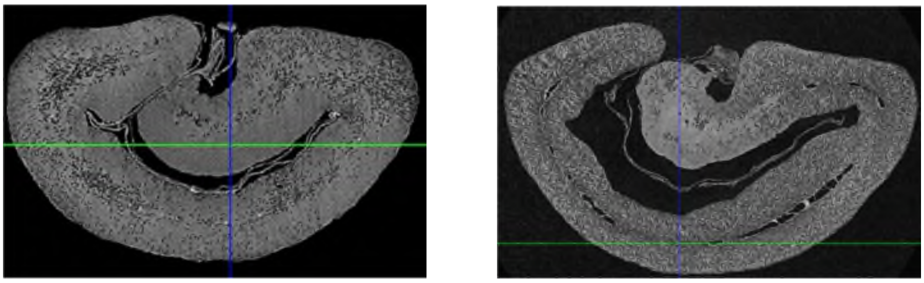

Figure 2: SEM images of a cross-section of a typical coffee bean before roasting (left) and after roasting (right). Image courtesy of Mondelez International.

In this report, we begin by discussing key issues that arise in the industrial process of roasting coffee beans. We first review an existing model for the roasting of a single coffee bean (Fabbri et al, [1]). Some shortcomings of the model are then discussed, which give rise to creating a mathematical model that overcomes these limitations. We then derive a model that incorporates the production of carbon dioxide gas, latent heat due to evaporation within the bean, multi-phase flow, and the changing porosity of the bean. We then made some simplifications in order to gain a preliminary understanding of the roasting process. Finally, we compare the results of our model with those presented in [1].

It is natural to question whether our model provides a better description of the coffee roasting process than those already in the literature, which already provide a reasonable fit to experimental data with a suitable choice of parameters. We examine the local moisture content with our model, in order to see whether the results agreed with previous results from the literature. At the end of this report, some recommendations and future tasks are discussed to develop the First Principles model further.

2. Previous Mathematical Models

One model that is already used by coffee manufacturers, such as Jacobs Douwe Egberts, is by Fabbri et al [1]. In this paper, a model for the roasting of a single bean is presented, which focuses on treating the temperature in the bean and the bulk moisture content. The model, however, has a number of simplifications that make it difficult to understand the values of certain parameters and equations. In particular, the authors assume that evaporation can only occur at the surface of the coffee bean, and no explicit phase change between liquid water and water vapour is ever mentioned.

Furthermore, they introduce a “mass diffusivity” term to describe the transport of moisture in the coffee bean that was originally derived from a paper focusing on the drying of coffee beans. However, they operate is in a parameter regime quite different from roasting, and in which the temperature of the bean is always below the boiling temperature of water. Nevertheless, the model presented in [1] is a good start to the modelling of coffee bean roasting, with parameters such as the moisture content of the bean treated as “lump” quantities. However, this also means that the “bulk” thermal properties of the bean were oversimplified for the roasting process, and that latent heat production and evaporation, which are local effects, cannot be sensibly incorporated.

3. New Models for Roasting of Single Beans

Our model is derived from mass and energy conservation equations while also including multi-phase flow.

We 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. We assume that no deformation of the bean occurs during the roasting process, and that the density of the solid coffee bean and the liquid water are constant.

As a preamble to multi-phase flow, we consider a representative small volume of interest with three phases present: solid (I), liquid (II), and gas (III). The solid phase comprises of cellulose and other organic molecules that make up the coffee bean. The liquid phase consists of only liquid water. Finally, in the gas phase, water vapour and CO_2 coexist within the same volume fraction. This can be summarized using Figure 3, where the volume of interest is shown within a black circle, with each phase marked.

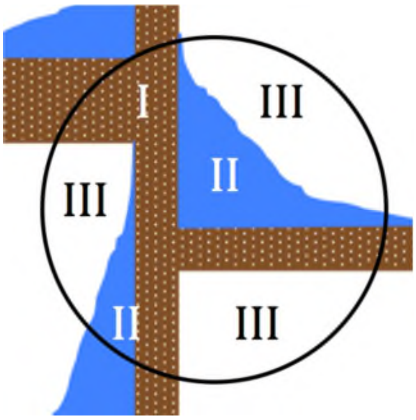

Figure 3: Representative volume of interest for multi-phase flow.

We assume that the cellulose walls degrade as the bean is roasting and produce CO_2, and that the liquid water evaporates. The rate of evaporation is related to the surface-area-to-volume ratio between phases II and III, and the molar mass of water, using the Langmuir equation [2]. Finally, we assume that the gases can freely move within the biological cells, as well as diffuse through the porous cell walls.

The dependent variables in our model are the porosity, water saturation, water vapour pressure, CO_2 pressure, and temperature.

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 and the degradation of the cell walls into CO_2. Finally, on the surface of the bean, we assume that heat is added to the bean in the roasting chamber by convection, and that the gas phases are held constant using Ideal Gas Law.

A visual representation of all of the processes described above is shown in Figure 4. 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.

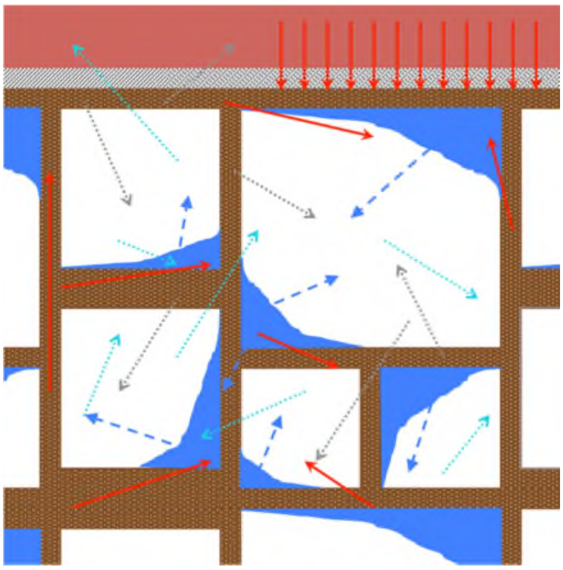

Figure 4: Schematic representation of the First Principles Model with all transport processes and boundary conditions shown.

Comments

- While our model gives us a strong description of processes relevant to the roasting of coffee beans, we were unable to find some parameter values in the literature, making it hard to properly analyse the model. In consequence, we are motivated to simplify the model to gain a preliminary understanding of its equations.
- We can simplify the model if we assume that CO_2 production is negligible and only consider water vapour in the gaseous phase, as well as assume that the porosity of the bean remains constant. These simplifications resolve any issues with not having all parameter values in the full model, and thus can be properly analysed using analytical and numerical techniques.
- This simplified model can then be solved in a spherical geometry and with radial symmetry. We took parameter values from the literature when possible, and consulted with JDE on appropriate values when they were not readily available.

4. Results

The simplified model predicts a “drying front” that propagates through to the centre of the bean. The model also predicts a “ridge” of built-up vapour pressure near the drying front.

We solved the simplified First Principles Model numerically, and present the results for the saturation, vapour pressure, and temperature in Figure 5. 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. In terms of water vapour pressure, we see a “ridge” of high water vapour pressure just before the drying front, which is then released into the roasting chamber in the dry region. Finally, we note that that the temperature in the coffee bean behaves nearly uniformly in space, and therefore suggests that we might approximate temperature as a function of time only.

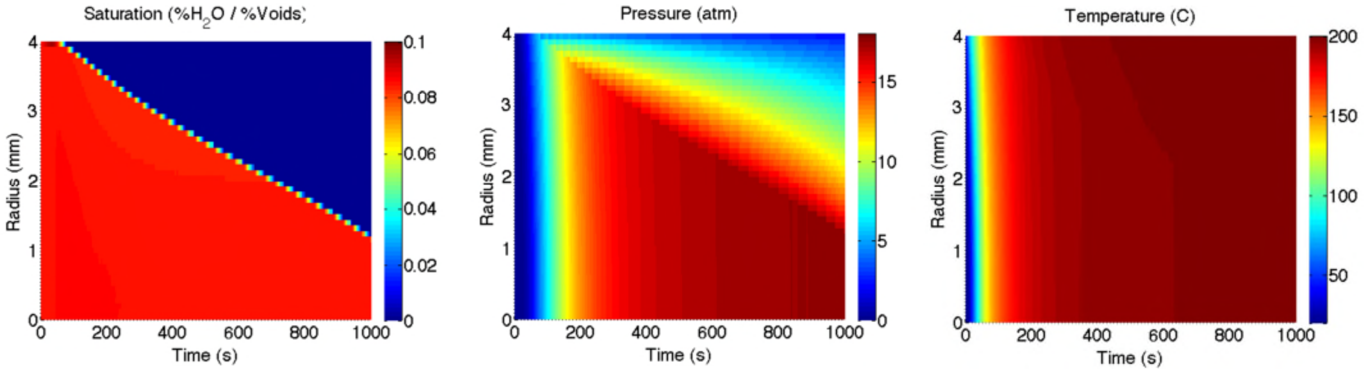

Figure 5: The Simplified First Principles Model for 1000 seconds of roasting at 200°C.

5. Comparison of Mathematical Models

A significant difference between the results in [1] and our simplified 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 [1], 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 simplified model, the coffee bean is distinctly divided into a moist region and a dry region. Additionally, the drying front in the simplified model moves more slowly than the model in [1]. We solved the model presented in [1] numerically on a spherical domain and compared this with the results of the simplified model. A comparison of the local moisture content in these two models is shown in Figure 6. While both models have been fit to display very similar average moisture concentrations in time (Figure 7), 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 [1] is entirely different from the region predicted by the simplified 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 [1] and our 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.

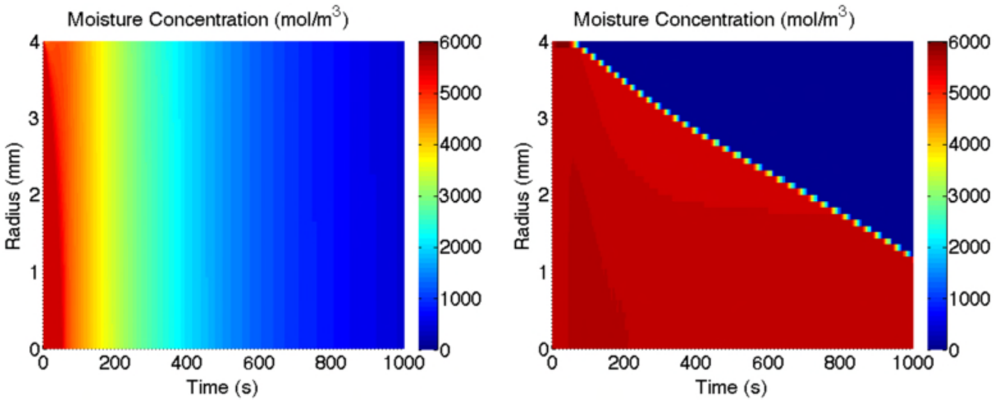

Figure 6: Comparison of the local moisture concentration for 1000 seconds of roasting at 200°C. The results using the model in [1] are shown on the left, and the results using our simplified model are shown on the right.

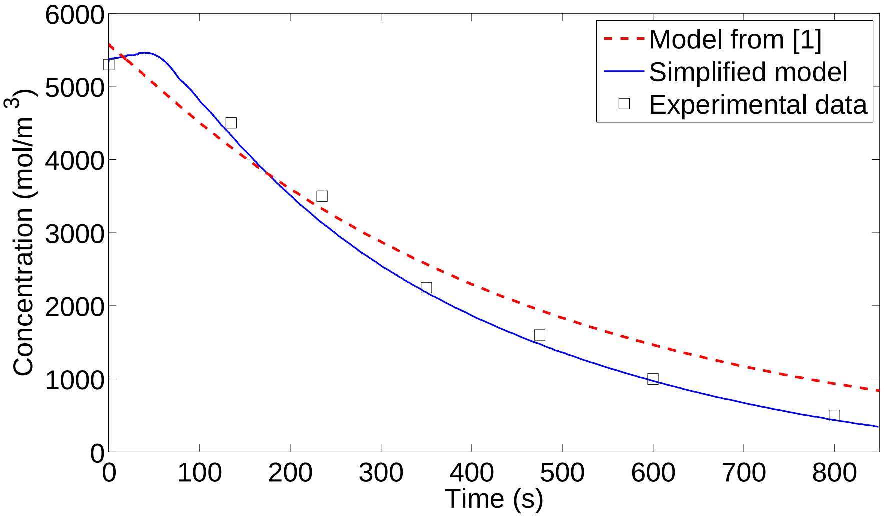

Figure 7: Comparison of the average moisture concentration for 850 seconds of roasting at 200°C, based on the model from [1], our simplified model, and experimental data reproduced from [1].

6. Conclusions and Future Work

We have built a mathematical model from first principles to describe the roasting of a coffee bean which incorporated, in a simple way, the porous structure of the bean. By simplifying the First Principles Model and fitting parameter values to experimental data, we were able to produce results similar to the experimental data presented in [1]. However, the model in [1] involed average moisture concentrations rather than local moisture concentration. In consequence, our 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 [1] was tailored to drying rather than roasting, we conclude that our model is better suited to understanding the roasting of coffee beans. Finally, the presence of a "drying front" that propagates towards the centre of the coffee bean is a key feature of the simplified model. This drying front seen in our results was not predicted in the model shown in [1], as their model uses average moisture concentrations rather than local moisture concentrations.

Future work on roasting will include:

- The numerical solution of our full model and a comparison with our simplified model
- Incorporation of deformation and solid mechanics
- Incorporation of the myriad of chemical reactions present in roasting coffee beans
- Further experimentation to improve parameter values and expand our models

Potential Impact

Alexandra Schulman and John Melrose of Jacobs Dowe Egberts commented on their experience collaborating with the CDT InFoMM program:

"Nabil has done a very successful project with Jacobs Douwe Egberts. The results have given us new and potentially important insights into the interior of a coffee bean during roasting which we will further investigate."

References

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

2. Langmuir, I. (1912). *The Vapor Pressure of Metallic Tungsten*. Physical Review **2**, 329-342.