EPSRC

Engineering and Physical Sciences Research Council

InFoMM

Industrially Focused Mathematical Modelling

EPSRC Centre for Doctoral Training in Industrially Focused Mathematical Modelling

A Critical Analysis of the Cereal Extrusion Process

Michael McPhail

UNIVERSITY OF OXFORD

Nestlé Research

Contents

1. Introduction

Extrusion with Vapour Expansion is a technique for producing large quantities of expanded food products ranging from breakfast cereals and snacks to pet food. Nestlé is interested in understanding the extrusion process better, since this is a technique that they use to make many of their products. A better understanding of how the final product depends on the design of the extruder and the input ingredients should result in more efficient trials and could potentially enhance production. An extruder (as illustrated in figure 1) consists of an inlet where raw materials are fed in, a screw system, and a die where the product exits. Within the extruder the screw, or screws, mix the raw ingredients and force them towards the die. The high shear exerted on the mixture as it moves down the extruder results in internal heating, and temperatures can reach up to 200°C. As the mixture reaches the end of the extruder it is pushed through a "die". As the mixture exits the die, the moisture dissolved within the mixture rapidly vaporises, resulting in the rapid expansion of the extrudate (the name given to the mixture leaving the extruder). This period of rapid expansion is called the "flash".

The "flash" is when the moisture dissolved within the extrudate vaporises, resulting in rapid expansion. This process is notoriously difficult to simulate.

The first step in understanding models for extrusion is to have a clear description of the composition of the extrudate. A mixture of starch-based powder (e.g. flour) and water is fed into the extruder and is mixed and cooked as it moves through the screw system. At the high pressures (~10 bar) achieved in the extruder, the water is dissolved within the cereal base (in this phase the dissolved water is called "moisture"). The pressure will drop as the mixture is pushed through the die until the pressure is too low to keep the moisture dissolved. The subsequent expansion as the moisture vaporises depends on the velocity of the extrudate, the pressure within the die, the quantity and dynamics of the moisture and the temperature within the extrudate.

The "screws" in an extruder (see fig. 1) push the cereal mixture through the extruder. As this happens, the high shear within the mixture results in significant internal heating, raising its temperature by up to 130 degrees

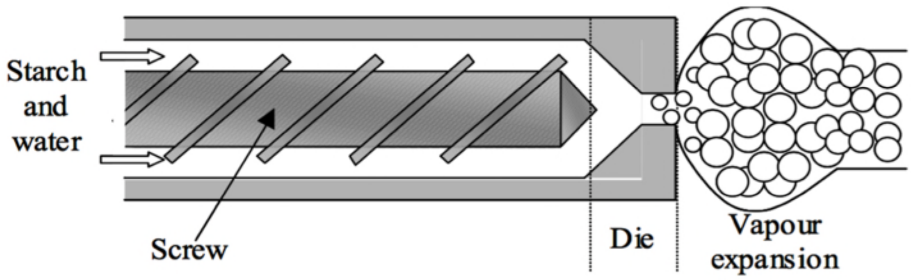

Figure 1: A schematic of the exit from an extruder. The mixture enters (from the left) and is at a high pressure with no vapour bubbles. As it moves to the right, bubbles form and expand.

Extrusion is very sensitive to changes in the system parameters such as the ratio of ingredients in the mixture, the die geometry and the ingredient feed rate. A reliable, efficient mathematical model for the extrusion process would serve as a very useful tool in the design of extrusion trials and eventually for the commercial production of extruded foods. The major difficulty in modelling extrusion is in simulating the "flash" as this occurs rapidly, produces large changes in the system, and is very sensitive to how the extruder is setup, and the mixture being used. Nestlé have previously sponsored a PhD in which a model for the extrusion process was developed [1]. Full numerical simulations of this model and a reduced model were carried out. The simplified (i.e. 1 dimensional) model was able to explain why, unexpectedly, adding more moisture to the mixture can result in a less expanded product. The unintuitive, yet important, results unearthed by a reduced model motivate the study of a full model. The additional complexity of simulating the full three dimensional system posed a number challenges to Lach [1], the most stifling being that the numerical simulations would not converge. Our aim is to review the model and the numerical scheme implemented by Lach [1], as well as developments in models for extrusion that have been published in the literature concerned with food production, multiscale modelling, and closely related physical phenomenon (including degassing of magma in volcanoes). Our goal is to build on the developments made in this field to be able to effectively simulate extrusion.

Before we begin simulating the flashing process, we want to make sure that the current model [1] is critically analysed. It is important to understand the assumptions that were made when this model was built, as these will play an important role in determining the parameter ranges for which the model is valid. Additionally, some of the assumptions made when this model was originally constructed that were intended to reduce the complexity of the system may now be unnecessary due to developments in the field since then.

2. A Model for the Flash

One difficult aspect of this problem is that the physical quantities vary throughout the extrudate on two very distinct length scales. The bubbles are initially very small (on the order of 10 microns; the "microscale") compared to the overall size of the extrudate (on the order of millimetres; the "macroscale"). A solution to this problem utilised by much of the literature on food science, and by Lach [1], is to model each lengthscale separately and then couple them together to form a multiscale model. A simple example of coupling a microscale model and a macroscale model that was utilised by Lach is to determine the bubble radius at each point within the extrudate based on the local conditions (such as pressure) and then use this bubble radius, together with the number of bubbles per unit volume of liquid, to determine the density of the extrudate on the macroscale. As the bubbles grow, the density of the extrudate decreases (i.e. the extrudate expands). However this coupling is a simplification of the full problem. A full coupling between microscale and macroscale requires determining what happens to the moisture, temperature and bubble size on the microscale to inform what happens to the density, moisture content, temperature and rheological properties of the extrudate on the macroscale. It is also clear that what happens to these quantities on the macroscale alters the local conditions at each point, and therefore impacts the microscale model for bubble growth.

Macroscale model

The model described in [1] comprises of a system of equations that determine the velocity ($\mathbf{u}$), the pressure (p), the temperature (T), and the moisture content (X) of the extrudate (in an averaged sense). Here it has been assumed that the extrudate can be treated as a single phase flow (rather than a gas phase and a liquid phase flowing together) which significantly simplifies the governing equations on the macroscopic system, but is also the reason we must also have a microscale model which which prescribes how the volume fraction of vapour within the extrudate changes. The velocity and pressure within the extrudate will be mediated by the transfer of mass and momentum. In the simplest model of the rheology of the extrudate, this transfer is governed by a set of differential equations called the compressible Navier Stokes equations. However, the complex rheological properties of the extrudate may, in practice, depend on the moisture content, temperature, and bubble volume. The temperature and moisture within the extrudate will (i) advect by the extrudate flow, (ii) diffuse as inhomogeneities in their respective profiles arise, and (iii) decrease as the bubbles grow or increase by viscous heating within the extrudate. This process is described by an advection-diffusion-reaction equation.

The solution domain changes significantly as the extrudate leaves the die because the extrudates' surface is now free to move. The die no longer confines the extrudate to axial expansion.

When a system is described by a set of differential equations, it is important that the right amount of information is prescribed on the boundaries. While the mixture is inside the die, the boundary will be the walls of die. At the die walls, we prescribe that the fluid will not move, a condition commonly known as "no-slip". Moisture in the extrudate cannot penetrate the material of the die, so a suitable boundary condition is to enforce no flux of moisture at the surface of the die. Finally, heat can penetrate the die, therefore, if we assume that the die's temperature is steady (it is losing heat to the atmosphere as fast as it gains heat from the extrudate) we enforce that the temperature of the extrudate is equal to the temperature of the die where they meet. Outside the die, the extrudate is free to expand in all directions. The extrudate's surface forms the boundary, within which our equations must now be solved. As this boundary is free, we impose a kinematic condition, which ensures the molten starch at the surface moves with the same velocity as the surface, and a dynamic condition, which expresses the fact that there is no external stress exerted on the surface. We also expect moisture to evaporate out of the extrudate at the surface, since the concentration of the water vapour in the surrounding atmosphere is lower. Finally, the rate at which heat leaves the extrudate from the surface is determined using a radiation condition.

Microscale model

The microscale model is concerned with how a bubble will grow given the local conditions surrounding it. Bubble growth is affected by: the rheological properties, the pressure, the moisture content, the temperature of the fluid surrounding the bubble, the amount of vapour in the bubble, and the temperature of this vapour. Two key modelling assumptions made at this stage are that the bubbles and the environment surrounding the bubbles are spherically symmetric, and that the bubbles are far enough apart that they do not interact. Both of these assumptions will tend to become invalid when the bubbles get too large or when the bubble density is too large.

Finding the growth rate of a bubble in a finite envelope of fluid limits the amount of heat and moisture that can

A common technique used for modelling microscale bubble growth is to consider the growth of a bubble surrounded by an "envelope" of liquid (see figure 2). The volume of fluid in this envelope is assumed to be equal for all bubbles throughout the fluid. The advantage of this method is that the amount of moisture and heat available for each bubble to consume as it grows is well defined. Each bubble only has access to the moisture and heat in the envelope of fluid surrounding it. This means that we must prescribe that no moisture or heat enters the fluid envelope from the surrounding bubbles. One potential issue with this description is the assumption that the bubble only affects the fluid within the envelope, which is a relatively small quantity when compared to the total amount of fluid actually contained in the extrudate.

The dynamics of moisture and heat transfer are governed by an advection-diffusion equation; on the microscale there are no significant sources or sinks of either moisture or heat. At the interface between the vapour in the gas bubble and the molten cereal, the moisture is assumed to be in equilibrium with the vapour. As the pressure in the bubble changes, which will happen if it expands and/or changes temperature, the position of this equilibrium will change, and moisture will be vaporised to maintain equilibrium. This equilibrium condition will be governed by Henry's law. Additionally, as moisture is vaporised, heat is consumed, resulting in a flux of heat out of the fluid at the bubble interface.

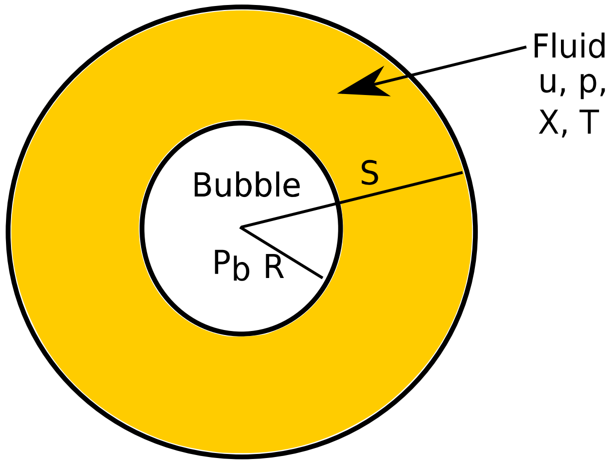

Figure 2: An "envelope" of fluid (yellow) of radius (S) surrounding a bubble of radius (R). Other unknown quantities include the pressure inside the bubble (P_b), the fluid velocity (u), the fluid pressure (p), the temperature within the fluid (T), and the concentration of moisture dissolved in the fluid (X).

The microscale problem is complex because the evolution of each variable depends on the current state of almost every other variable (highly coupled), every equation must be solved at the same time.

The rate of bubble growth is dependent on the pressure inside the bubble. The pressure will change as more moisture vaporises, as the temperature of the bubble changes, and as the size of the bubble changes. The simplest relationship between these quantities is known as the ideal gas law:

$$P_b = \frac{NR_gT}{V},$$

where P_b is the pressure in the bubble, N is the number of moles of gas in the bubble, R_g is a constant known as the "ideal gas constant", T is the bubble temperature, and V is the bubble volume. The ideal gas law illustrates the complexity of the coupling between the different processes, even on the microscale. The pressure depends on how much moisture has been vaporised into the bubble (through N), as well as the energy consumed in vaporising this moisture (through T). However, the rate at which moisture is vaporised, and energy consumed, will depend on the pressure in the bubble through Henry's law. Finally, the pressure in the bubble depends on the volume of the bubble, and the growth of the bubble radius depends on the pressure in the bubble.

Micro/Macro coupling

One aspect of the relationship between the microscale and macroscale models is how "information" is passed between them. For example, if heat is consumed by a bubble as it grows, how does this effect the temperature of the macroscale? This aspect was not considered in the previous model for bubbly flow [1], however as our approach involves mathematically defining all of the processes before implementation, we consider it now. One mechanism by which these two models may be coupled is to represent the growth of each bubble on the microscale as a sink of heat and moisture on the macroscale where the flux into bubble (or across some surface at some distance away from the bubble) on the microscale is the rate at which these quantities decrease on the macroscale.

Glossary of terms

- Advection: The transport of quantity by a moving fluid.
- Diffusion: The movement of a substance from a region of high concentration to a region of lower concentration. A substance with a higher diffusivity (D) will diffuse faster than a substance with a lower diffusivity.
- Rheology: Relates to how a material (e.g. a fluid) will deform under stress. For example: the rate of deformation of a Newtonian fluid will be linearly proportional to the stresses throughout the fluid.
- Viscosity: A measure of a fluids resistance to deformation.

3. Important processes

Because the Reynolds number (Re) is so small we can neglect inertia. As the Péclet (Pe) numbers for macroscale heat and moisture transport are large we can neglect the diffusion of these quantities.

The model described in the previous section captures the relevant physical processes for extrusion, most of which depend on the state of a number of variables within the system. By scaling the equations, determining the important dimensionless parameters and their typical sizes, we can systematically determine the processes that will not significantly affect the dynamics of the system. Some important dimensionless parameters for this system, and their approximate sizes, can be found in Table 1. The Reynolds number is the ratio of the fluid's inertia to its viscous stress and is small on both macroscopic and microscopic lengthscales. This means the fluids inertia will not play a significant role in the dynamics of the system. Therefore, we can safely neglect the inertia terms in the Navier-Stokes equations.

The Péclet number is the ratio of the diffusive timescale to the advective timescale. A large Péclet number means that diffusion is slow relative to the speed at which the fluid is flowing, and therefore it is a good approximation to ignore diffusive effects except possibly close to boundaries. The Péclet numbers for both heat and moisture transfer on the macroscale are large. This means that the extrudate flows too fast, over the typical lengthscales we consider, for diffusion to have any impact over macroscopic lengthscales. Hence, diffusion of heat and moisture may be safely ignored in the macroscale problem (except possibly close to the boundaries). This means that the advection-diffusion-reaction equations for heat and moisture transport on the macroscale reduce to advection-reaction equations where bubble growth will dictate how fast these quantities drop from their initial values within the die to the values they take at steady state on the macroscale.

Parameter	Reynolds (Macro-)	Reynolds (Micro-)	Péclet (Macro-, moisture)	Péclet (Macro-, heat)
Value	10^{-4}	10^{-9}	10^{7}	10^{4}

Table 1: Typical orders of magnitude for some dimensionless parameters.

4. Discussion, Conclusions and Recommendations

Our goal was to critique models for the flash that occurs as extrudate leaves an extruder. A critical part of this process is to identify the key assumptions that have been made in current models and determine whether they are both valid and necessary. To illustrate a particular model for microscale bubble growth, the cell model, in which a bubble's growth is affected only by an envelope of surrounding it, was considered. The cell model has the advantage of being a conceptually simple way of limiting the resources (such as heat and moisture) available to each bubble, although the assumption that the bubble is surrounded by a small finite amount of fluid is completely artificial. Through the assessment of important dimensionless parameters, additional assumptions can be incorporated to simplify the system being considered. One such assumption is to ignore the fluid's inertia, which simplifies the model for the flow of the extrudate.

As full simulations of extrusion are our final goal, the next stage is to begin a numerical implementation of this model. Alongside this approach, systematic simplifications of the model can be identified (in particular regimes) which might make analytic progress tractable. The benefit of pursuing an analytic approach is that it can serve as a comparative tool by which future numerical simulations can be tested. One avenue to making numerical simulations easier is to try and express bubble growth entirely in terms of macroscopic variables. By using asymptotics to find the leading-order problem on the microscale, which features only ODEs and integral equations, we no longer need to solve microscale PDEs coupled to macroscale PDEs. This would make full simulations more tractable as the complexity in the system is now confined to the macroscale problem.

5. Potential Impact

Ritchie Parker, Process Modelling Group Manager, Nestlé PTC Orbe said *"Vapour flash and gas expansion of viscous fluids are important in many food processes, especially for extrusion, so the development of a robust model of vapour expanded extrusion should lead to a better understanding of how these processes work and help us to optimise process design to produce porous products with the right texture and shape to delight our customers. I am particularly excited by the simplifications currently being developed through asymptotic analysis of the microscopic equations which should allow a robust simulation of the early expansion phase and the possibility for simple coupling with an industrial CFD code.*

There are, however, many additional physical phenomena to address before we can model the complete process, including nucleation, bubble interaction, breakup and coalescence. Many properties that the process depends on, such as product rheology, water activity, mass and heat diffusivities are functions of temperature, moisture content and other conditions that evolve during the process, so we cannot expect to make accurate predictions in the short term. But in the medium to long term I believe this work has the potential to produce a reliable simulation tool that can help product developers and engineers design expanding food processes faster and with greater reliability than is presently possible."

References

1. L Lach (2006) *Modelling Vapor Expansion of Extruded Cereals*. PhD thesis.