Modelling the mixing process of liquids with concentrates in capsules

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MODELLING THE MIXING PROCESS OF LIQUIDS WITH CONCENTRATES IN CAPSULES

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ABSTRACT

In food industry mixing of concentrates contained in capsules with liquids such as milk or water for the production of warm drinks is becoming common practice the last couple of years. This process is characterized by complicated physical phenomena: the concentrates' viscosity is temperature dependent, the liquid is non-Newtonian and the mixing process is turbulent. The industrial objective at the end of the process is a uniform liquid end product with as little as possible left over concentrate in the capsule. The optimization of the mixing process is typically done by trial and error in laboratories, which is time consuming and expensive. Computer models can significantly reduce the manufacturing costs associated with laboratory optimization and give a better insight of the process. The objective of this paper is to create a computer simulation model that is able to capture the physical processes occurring during the production of warm drinks using finite elements. The model should be able to correctly represent the mixing of the solid concentrate with the liquid injected inside the capsule compartment. Finite element method is used to solve the flow, heat exchange and concentration problem. In the paper different shapes of the capsule and how they influence the mixing are compared and their suitability for industry according to the amount of concentrate left in the capsule at the end of the process are assessed.

Key words: food processing, mixing, turbulence, multiphase flow, finite elements

NOMENCLATURE

c	kg/m^3	concentration
D	m^2/s	diffusion rate
c_p	J/kgK	specific heat
f	m/s^2	body force (gravitation)
k_c	W/mK	conductivity
p	Pa	pressure
t	sec	time
U	m/s	velocity
μ	m^2/s	dynamic viscosity
ρ	kg/m^3	density

σ Pa Cauchy stress tensor

INTRODUCTION

Hot beverage brewing apparatuses have become an integral part of every day life. A variety of them exists often as merchandisers for brewing and selling predetermined amounts of hot beverages of various types: coffee, tea, hot chocolate, cappuccino, soup, etc. The last couple of years the use of disposable portion capsules for the preparations of beverages has become ever more popular since they provide a desirable end product for the consumer with minimum effort, short time preparation and minimum after-use maintenance.

Encapsulation involves the incorporation or entrapment of necessary ingredients (pure material or a mixture into another material) that can dissolve in water for the beverage preparation in a capsule or carrier or shell. Since production volumes have increased and more cost-effective preparation techniques and materials have been developed, the number of encapsulated food products has significantly increased. The capsule protects the content from the environment which can be destructive while it can allow with the use of membranes the passage of water. The design of the capsule is very important for the quality of the end beverage.

Usually the water enters the capsules chamber through a membrane on one side of the capsules and the end product exits on another side. A variety of microchannels through osmosis can assist the mixing of the encapsulated ingredients with the dissolvent water as it passes through the capsule and drags along the main beverage ingredients. The capsule design should be such that: it can store the ingredients needed for the beverage preparation in an aroma-tight compartment; it can allow through the membrane the water to enter the compartment and guarantee a uniform, good brewing result; the remaining residual inside the capsule after brewing should be minimum; and the disposal of the capsule is non-problematic and clean.

The design optimization of new methods and products in the food industry is usually performed by trial and error experimentation in research laboratories. There are major drawbacks related to this approach. Experiments are often time consuming and costly and at the same time only a restricted

number of variable or designs can be used for control and optimization.

The use of computer aided technologies such as computer modeling for design optimization is beneficial to industries as it results in lower product development costs and a greatly shortened design cycle. The last thirty years computer modeling is widely used in several industries i.e automotive, aerospace, nuclear, in a variety of applications. Only in recent years it has been used in food industry [1-4] to better understand the complex physical mechanisms: thermal, physical, rheological, material properties that govern food processing. It has been used to model a variety of topics including modeling oral processing of foods [7]. Reviews of the use of computational modeling in the food industry can be found in [2-6]. Computational models can be used as a tool to predict food processing as well as to design food processing equipment before it is even manufactured or implemented. Applications in the food industry include drying [8,9], sterilization [10], refrigeration [11,12], mixing [13-14].

As mentioned above mixing is an important area and one of the most common operations for the preparation of food and beverages and it involves substances of gas, liquid and solid. Modeling mixing is not an easy task, it involves complex physical phenomena such as turbulence, multiphase flows, temperature depended viscosities, non-Newtonian fluids and it strongly depends on the shape of the mixer. The design of the mixing devise is an important part in analyzing the mixing process. Many researchers have focused on using computational modeling for the design of the mixing devises for the food industry [13, 14].

Traditionally mixing has been achieved by stirring and is used in food production lines in factories [15]. They make use of the baffled-imposed turbulence to provide mixing. For modeling this process, the computations need to embed turbulence models capable of capturing the underlying process. In cases where a stirrer is difficult to be present and small scales are involved the most favorable alternative to stirring is the static mixer approach which is accomplished mainly through diffusion. Static mixers do not require a moving part and external agitation. Mixing is achieved by the natural motion of the fluid as it flows through the mixing elements of the static mixer.

The objective of this paper is to model the mixing process of water with the viscous liquid ingredients inside a capsule for the preparation of hot beverages. The industrial aim is to obtain an optimal design of the capsule and the channels inside the capsule that produce a uniform mixing of the drink and leaves as little as possible residual behind in the capsule after the end of the mixing. The finite element model should be able accurately capture the process and give information relate to flow profile inside the capsule and the concentration field with time for various capsule designs.

MATERIALS AND METHODS

1. Beverage preparation

The beverage mixture starts as a dense concentrate inside the capsule. The capsule's shape is shown in Figure 1 where at the top of the capsule there is a foil used to seal the content

inside. This foil is removed before the capsule is placed in the beverage apparatus. Below the foil there is a membrane which still seals the capsule but is permeable through small holes which allow the water to pass through, without allowing the content of the capsule to come out. When the capsule is placed at the beverage apparatus a hole is made at the bottom of the capsule in order to allow the beverage to come out. Hot pressurized water is injected at the top of the capsule by the beverage apparatus. The water is entering the capsule compartments A and B. The concentrate which resides in these two compartments is dissolved in the water and through osmosis is diffused and travels through the capsules channels to finally exit at the bottom of the capsule. A schematic representation this is shown in Figure 2.

Figure 1: Capsule.

Figure 2: Schematic representation of the flow within a capsule.

2. Governing Equations

This section is concerned with presenting the mathematical model used to describe the mixing of water with the thick concentrate inside the capsule. It involves the motion of the fluid inside the capsule, the heat exchange occurring and the change of the concentration when the water is mixing with the thick concentrate.

Flow problem

The governing equations of the fluid flow for an incompressible Newtonian fluid are described by the continuity and the momentum equation.

Continuity equation or mass conservation:

$$\nabla \cdot \mathbf{U} = 0. \quad (1)$$

Momentum equation:

$$\rho \left(\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot (\mathbf{U}\mathbf{U}) \right) = \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{f} \quad (2)$$

For Newtonian fluids the constitutive equation for the stress tensor, $\boldsymbol{\sigma}$ is given by:

$$\boldsymbol{\sigma} = 2\mu \text{dev}(\dot{\boldsymbol{\varepsilon}}) - p\mathbf{I} = \mu (\nabla \mathbf{U} + \nabla \mathbf{U}^T) - p\mathbf{I} \quad (3)$$

where $\boldsymbol{\varepsilon}$ is the strain tensor, $\dot{\boldsymbol{\varepsilon}}$ is the strain rate tensor and $\text{dev}(\cdot)$ is the deviatoric part of the tensor. The dynamic viscosity depends on the temperature and the concentration $\mu := \mu(T, c)$. It is given by

$$\mu = \mu_\infty + \frac{\mu_0 - \mu_\infty}{1 + K \dot{\gamma}} \quad (4)$$

where $\dot{\gamma} = \nabla \mathbf{U} + (\nabla \mathbf{U})^T$.

Substituting (3) into (1) the momentum equation can be rewritten as:

$$\rho \frac{\partial \mathbf{U}}{\partial t} = \nabla \cdot (\mu \nabla \mathbf{U}) - \rho \nabla \cdot (\mathbf{U}\mathbf{U}) - \nabla p + \rho \mathbf{f} \quad (5)$$

Heat exchange

The heat flow can be described by the energy equation and for an incompressible fluid in a Eulerian description it reads

$$\rho c_p \left(\frac{\partial T}{\partial t} + \mathbf{U} \cdot \nabla T \right) = k \nabla^2 T + \mu [\nabla \mathbf{U} + (\nabla \mathbf{U})^T] : \nabla \mathbf{U} \quad (6)$$

Concentration

The fluid is defined at any point in time and space as the concentration c , defined as the beverage concentrate to water fraction, going from 0 to 1, i.e. from pure water to the dense concentrate. The evolution in time can be described by a convection-diffusion equation.

Convection diffusion equation

$$\frac{dc}{dt} + \mathbf{u} \cdot \nabla c = \nabla \cdot (D \nabla c) \quad (7)$$

where $\mathbf{u}$ is the speed vector and D is the diffusion rate.

3. Computer Simulation Model

The finite element method has been used for the discretisation of the Stokes problem, the convection-diffusion equation. The finite element formulation has been implemented in COMSOL with matlab [16].

For the simulations a 2D simplified case was considered and a full 3D case. For the 2D case only the flow between the first two compartments was studied. This simplified representation is enough to capture the phenomena occurring without lengthy computation. For the 3D case the problem can be solved as axi-symmetric using a 60° degrees wedge of the capsule. For the 3D case two different geometries were modeled as the shape of the capsule is important for the end product. An unstructured mesh was used for the computations; the mesh for the 3D case is shown in Figure 3 for Shape A and Shape B. The mesh is coarser at the top holes where the water enters the capsule, at the connecting channel between the different compartments and at the outflow.

Figure 3: Mesh of the 60° wedge of the capsule.

The boundary conditions for the heat exchange are fixed temperature at the inlets, completely insulating boundaries and no gradient at the exit. The walls of the capsule are treated as insulating. For solving the concentration problem it is considered that the sides of the container are not permeable by the fluid so

$$-D(\mathbf{n} \cdot \nabla c) + c(\mathbf{n} \cdot \mathbf{U}) = 0 \quad (8)$$

On the inflow boundaries, pure water is injected, which can be written simply as $c=1$. Finally, the outlet is a free outlet assuming that the concentration does not change anymore near the exit and is modeled as

$$-D(\mathbf{n} \cdot \nabla c) = 0 \quad (9)$$

RESULTS

The dependence of the viscosity with temperature of the concentrate as it is mixed with water for different temperatures of water ($20^0, 40^0, 60^0$) is shown in Figure 4. This data is obtained experimentally. For industrial secrecy the actual values are not shown.

Figure 4: Concentrates viscosity changes with time for different temperatures.

In the beverage apparatus the water is passing through the capsule in a time window of 40s. The 2D dummy test case was used to be able to have an overview of the main effects in compartments A and B where the concentrate resides. The change of the concentration inside the two compartments and the velocity field can be seen in Figure 5 for $t=0.2, 1, 3, 5$ s. It can be seen that the concentrate mixes and leaves the compartment B faster than in compartment A.

Figure 5: 2D dummy. Change of concentration and velocity field stream lines in the cup at times 0.25, 1, 3, 5 s. Red is 100% concentrate and blue is 100% water.

For Shape A the change of concentration inside the capsule at different times $t=0.25, 5, 15, 20, 30, 40$ s is shown in Figure 6. In the figure brown is representing 100% concentrate and white is 100% water. The concentrate is mixing with water and exits the capsule in 40 s and traces of residue are left in the capsule. The observation from the 2D case that the concentrate leaves the compartment B faster than compartment A is also seen in the 3D case.

Figure 6: Shape A. Change of concentration in the cup at times 0.25, 5, 15, 20, 30, 40 s. Brown is 100% concentrate and white is 100% water.

The change of the concentration of the beverage exiting the outlet of the capsule against time can be seen in Figure 7. The flow cannot be considered as two phase flow, or as a flow encompassed by two separate fluids. Before the process starts two separate fluids can be considered: the boiling water in the machine and the cold concentrate in the cup. The moment the water enters the cup, some of the concentrate will diffuse in it instantaneously. Therefore within the cup one can only consider the flow as one among infinitely many different fluids, or more conveniently, as a single fluid with varying concentration and varying physical properties depending on that concentration. Within the cup concentrate is diffused such that at no single location one could possibly discern an objective boundary between two different fluids. Given a parcel within the cup during the process, one cannot simply say it is part of a fluid 1 or a fluid 2; one can only state how much of fluid 1 and fluid 2 has been mixed to arrive at the same physical state as the liquid within that parcel.

Figure 7: Shape A. Concentration vs Time at the exit.

The flow streamlines between compartment A and compartment B can be seen in Figure 8.

Figure 8: Flow stream lines in 3D case.

In order to study the role of the inner compartments in the mixing process two cases were considered: Case 1: with inlet holes in the top of the inner compartment creating a flow through that inner compartment. This flow enhances the working of the cup; Case 2: without inlet holes. This prevents flow within the inner compartment. The change of the concentration of the beverage inside the capsule against time can be seen in Figure 11. The left hand side shows Case A at different times and the right hand side shows Case B. The concentration changes as the water is mixed with the concentrate and from 100% concentrate becomes less dense concentrate mixture. From the computations it is shown that the purpose of the inner compartment is that of enhancing the concentration at the exit of the cup.

In Figure 9 the concentration of three points in the cup is shown. The blue line depicts a point inside the inner compartment, the green line a point in the outer compartment, and finally the red line a point near the exit. The concentration at the exit is regularized by the presence of the inner compartment.

Figure 9: Shape B. Case A and Case B. Change of concentration of three points in the cup.

The pressure and the velocity at two points are shown in Figure 10. The blue line depicts a point inside the inner compartment, the green line a point in the outer compartment. Pressure difference behavior is clearly not different in the two cases, after a numerical start-up effect. The difference in the shape of the pressure curve at around 20 seconds can be explained by the fact that the downstream viscosity is lower for case A. Speed shows similar behavior at all points.

Figure 10: Shape B. Case A and Case B. Change of pressure and velocity at two points in the cup.

Figure 11: Shape B. Case A and Case B. Change of concentration during mixing for case A and B. Red is 100% concentrate and blue is 100% water.

The working of the cup is not enhanced by an under-pressure near the hole between the inner and outer compartments, but rather by the lowering of the viscosity of the upstream mixture. The pressure drop is caused by the well known Venturi effect and the Bernoulli law. The driving force of the flow in the capsule is the imposed pressure difference between top and bottom of the cup — the cost of the hot beverage machinery largely comes from the equipment needed to impose such a pressure difference. But even then, we have shown a similarity between case 1 and case 2 where there is hardly any difference in behavior of the pressure drop (and related speed up) near the hole between the compartments, while the flow inside the inner compartment is of a completely different nature. In case 1 there is a flow of fluid 2 (water), while in case 2 there is an unmoving bulk of fluid 1 (concentrate). From case 2 and specifically the fact that the concentrate is stationary, it can be seen, that there is not much transfer of momentum between the different levels of concentration.

While the flow of the outer compartment to the exit of the capsule is largely autonomous, i.e. it is driven by the imposed high pressure at the top and the lower exit pressure. The inner tube provides an additional, second order, effect. It allows to empty itself quickly, due to its smaller volume and relatively large concentration of inlet holes. Because the flow below the inlet holes, and consequently through the inlet holes is fast, the pressure drop through the inlet holes is larger. This allows a smaller pressure in the inner compartment. Secondly, it dilutes faster, as more concentrated fluid is pushed out, and a less concentrated mix is created in this compartment. This more diluted mix is pushed out, together with the denser fluid from the outer compartment. This means that a more diluted mix reaches the mixing stage of the cup more quickly, and allowing a more gradual change in concentration during the brew.

CONCLUSIONS

In this paper the mixing of a concentrate with water inside a capsule for the preparation of hot beverages was presented. The problem was modeled using finite elements methods. The phenomena occurring during the mixing were modeled by solving a flow, heat and concentration problem. The change of concentration during the mixing can be accurately represented by using the convection diffusion equation without the need to model the problem as a two phase flow. The computer modeling presented in this paper can be used for industrial applications in mixing beverages in capsules. It can be used to give a better insight of the rheological process occurring in the preparation of the beverage and help to optimize and control the design of capsules.

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