Numerical Solution of a Model Associated with the Production of Hollow Micro-particles

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Abstract

Fundamental models of engineering processes frequently lead to systems of partial differential equations with free boundaries. Examples include crystal growth and biofilm growth where the boundary is not known a priori, but has to be determined as part of the numerical solution. A sub-class of these problems are ones in which the position of the boundary changes as a function of time. This work primarily addresses the numerical solution of a spray drying process that produces polymeric hollow micro-particles.

A solution, which contains the polymer and a blowing agent is atomized into the drying chamber and brought in contact with a hot air stream. The blowing agent, which is trapped in the droplets, decomposes at higher temperatures creating a void in the center of the particle. Since the air stream temperature is greater than that of the droplet, the droplet temperature increases until the evaporation temperature of the solvent is reached. The solvent at the surface begins to evaporate causing the solvent below the surface of the droplet to diffuse to the surface. Simultaneously, the blowing agent that is a part of the droplet begins to decompose. As the solvent evaporates, the droplet shrinks and as the decomposition reaction occurs, the droplet expands. If these processes are balanced, the droplet, as it passes through the spray chamber will form a hollow particle. If, however the rate of the decomposition of the blowing agent is greater than the rate of shrinkage of the droplet, then the formed particles will collapse. On the other hand, if rate of the decomposition of the blowing agent is much smaller than the rate of shrinking of droplet, the particles will not be hollow. The starting point of the model is the formation of a single hollow micro-particle from a single droplet of the feed solution. The fundamental model obtained is in the form of a set of parabolic PDEs with a moving boundary at the surface.

Numerical approaches to address moving boundary problem can be classified as 1) front tracking ,2) front fixing or 3) fixed domain methods. In the front tracking method, the position of the boundary is solved leading to unequal grid spacing. The front fixing method ,on the other hand, employs suitable transformations to fix the position of the boundary in the transformed domain. One drawback of this method is that if the position of the boundary does not appear explicitly in the equations then an estimate of the boundary must be provided. If the boundary does not change smoothly or monotonically, the entire domain is fixed and the boundary condition is found implicitly. This is the fixed domain method.

This work considers two front tracking methods, the modified variable time-step (MVTS) finite difference method [1] and the Moving Finite Element method (MFE) [2] to solve the moving boundary surface associated with the formation of polymeric micro-particles. Finite difference methods have been used to solve moving boundary

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problems. Variable step finite difference methods were introduced primarily to avoid estimation of the position of the boundary, which was a drawback of the fixed grid methods, and therefore improve the accuracy of the solution.

The variable time-step method in its original form updates the time step such that the boundary was at a grid point at all the points. However, this led to an instability, which was addressed by the MVTS method by updating the time step based on the boundary condition. An implicit finite difference method is used, which requires a recursive algorithm at every time step. Additionally, the MVTS method facilitates the solution of implicit moving boundary problems.

The MFE method is an adaptive griding finite element method that has been shown to be suitable for solving PDE systems with a moving boundary [3]. A distinguishing feature of the MFE is the concept of nodal movement. Whereas in the traditional finite element methods a single set of *basis* functions is defined, the MFE introduces a second set of basis functions to account for the movement of the nodes. The second set of basis functions, which is related to the first set, is then used to generate a residual function, similar to the residual obtained from the first basis function. Both residuals are minimized simultaneously to provide a value of the dependent variable and the position of the nodes. This method however, requires solving twice the number of equations but it also has double the number of degrees of freedom and thus provides greater flexibility than the regular finite element method. The accuracy of the MFE solution will be compared to the finite difference solution using the model developed for the production of a hollow micro-particle from a spray drying process.

References

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