Modeling the Production of Hollow Micro-particles

Vikram Shabde, Uzi Mann and Karlene Hoo
Department of Chemical Engineering, Texas Tech University

Objectives

- Propose a fundamental model for skin formation
- Validate model against experimental results

Motivation

- Hollow particles have a number of applications, such as syntactic foams.
- Drug delivery is another application where hollow micro-particles can be used.

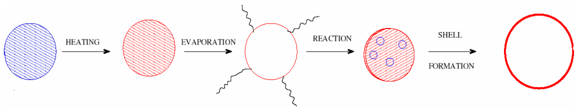

Fig.1 : Different phenomena occurring as the droplet passes through the spraying chamber.

Process Description

The experimental setup consists of a cylindrical chamber in which, a solution of the polymer is sprayed. The solution is made by dissolving the polymer and a "blowing agent" in the solvent. Hot air is circulated along with the spray. The hot air also heats the droplets. Evaporation of the solvent, decomposition of the blowing agent and curing of the polymer lead to the formation of hollow particles. Fig. 1 shows the phenomena occurring as a droplet passes through the chamber. Fig. 2a and 2b shows the shape of the micro-particles.

Fig.2a: SEM of the micro-particles.

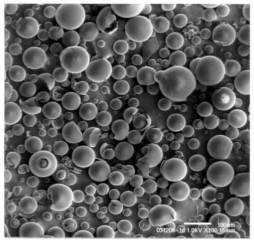

Fig.2b: Optical image(67.8mm).

Model

The model developed considers the heating of the droplet and evaporation of the solvent from the droplet to form the skin. Fig. 3 shows the proposed mechanism for solvent and polymer transport within the droplet. Water is chosen as the solvent. It is proposed that Fickian diffusion of the water and polymer within the droplet occurs while heat transfer follows Fourier's law of heat conduction[2]. Since the relative velocity of an individual droplet is quite small the heat transfer coefficient is high. Thus in the model, the loss of water due to mass transfer is neglected and only the loss due to the heat transferred is considered. Since the droplet travels through two zones, the heating zone and the evaporation zone there are two sets of boundary conditions at the surface of the droplet. In the first zone, the heat transferred from the air to the droplet is modeled using a convective heat transfer relationship. In the second zone, the solvent evaporates and this causes the surface of the droplet to recede which give rise to a moving boundary at the surface. As a result of the moving boundary, there is an additional condition describing the boundary velocity.

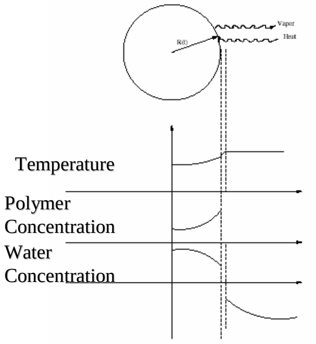

Fig.3: Water & polymer transport.

Water Diffusion

$$\frac{\partial \bar{c}_W}{\partial \tau}=\frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\frac{\partial \bar{c}_W}{\partial x}\right) \quad 0 \le x(\tau) \le X(\tau)$$

Polymer Diffusion

$$\frac{\partial \bar{c}_P}{\partial \tau}=\frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\frac{\partial \bar{c}_P}{\partial x}\right) \quad 0 \le x(\tau) \le X(\tau)$$

Heat Diffusion

$$\frac{\partial \theta}{\partial \tau}=Le\frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\frac{\partial \theta}{\partial x}\right) \quad 0 \le x(\tau) \le X(\tau)$$

Boundary Conditions

Heating

$$\frac{\partial \bar{c}_W}{\partial x}\left(X(\tau),\tau\right)=0$$

$$\frac{\partial \bar{c}_P}{\partial x}\left(X(\tau),\tau\right)=0$$

$$\frac{\partial \theta}{\partial x}\left(X(\tau),\tau\right)=Le\cdot H_{evap}\cdot Bi\left(\theta_{air}-\theta\left(X(\tau)\right)\right)$$

$$X(\tau)=X(0)$$

Evaporation

$$\frac{\partial \bar{c}_W}{\partial x}\left(X(\tau),\tau\right)=\left(1-\bar{c}_W\right)\frac{\partial X}{\partial \tau}$$

$$\frac{\partial \bar{c}_P}{\partial x}\left(X(\tau),\tau\right)=-\bar{c}_P\frac{\partial X}{\partial \tau}$$

$$\theta\left(X(\tau),\tau\right)=\theta_{sat}$$

$$\frac{\partial X}{\partial \tau}=Le\cdot H_{evap}\left(Bi\left(\theta_{air}-\theta\left(X(\tau)\right)\right)-\left.\frac{\partial \theta}{\partial x}\right|_{x=X(\tau)}\right)$$

Numerical Method

The Gradient Weighted Moving Finite Element Method[3] is used to solve the model equations. The method is a moving node technique and thus the boundary velocity can be explicitly found.

Results

Fig.4 shows the polymer concentration within the droplet at different times. A "skin" is said to have been formed. when the polymer concentration reaches 100% on the surface of the droplet.

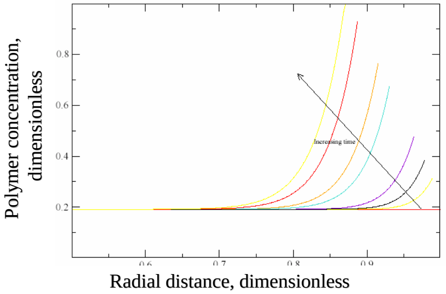

Fig.4: Polymer concentration within the droplet.

Fig.5 shows that for a 25% uncertainty in the heat transfer coefficient the time to skin formation varies inversely with the heat transfer coefficient.

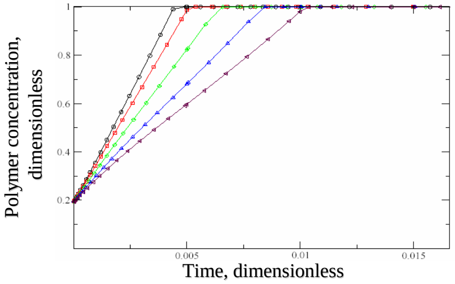

Fig.5: Heat transfer coefficient effect.

References
1) Wilcox, D. and Berg, M. (1994) Material Research Society, Proceedings, **572**.
2) Bird, B. , Stewart, W., and Lightfoot, E. (2002) "Transport Phenomena" Wiley, NY.
3) Miller, K. and Carlson, N. (1998) SIAM J. Num. Ana, **19**(3).