Droplet Models Useful for Pharmaceutical Particle Precipitation Simulation

Research and Teaching Repository

Background

- Models of determination of droplet heating and vaporization rates are critical for spray problem modeling in various applications, such as pharmaceutical particle precipitation.
- After implementing the droplet heating and vaporization models and other relevant models, CFD is a very powerful tool to predict features and performance of many processes, e.g. morphology of biomedical spray-dried polymer particles.

Types of droplet-vaporization models

- Constant-droplet temperature model
- Infinite-liquid-conductivity model (the type of the following listed models)
- Spherically symmetric transient droplet heating (or conduction-limit) model
- Effective-conductivity model
- Vortex model of droplet heating
- Navier-Stokes solution

Ranz and Marshall model

The dimensionless number determining the droplet heating and vaporization rate, i.e. Nusselt number Nu and Sherwood number Sh are give by:

$$Nu = \frac{hd_p}{k_\infty} = 2.0 + \beta_c Re^{\frac{1}{2}} Pr^{\frac{1}{3}}$$

$$Sh = \frac{h_m d_p}{D_{v,m}} = 2.0 + \beta_c Re^{\frac{1}{2}} Sc^{\frac{1}{3}}$$

Spalding number correction

The models with Spalding number correction are more accurate in vaporizing cases.

$$Nu = \frac{hd_p}{k_\infty} = \frac{ln(1 + B_M)}{B_M}\left(2.0 + \beta_c Re^{\frac{1}{2}} Pr^{\frac{1}{3}}\right)$$

$$Sh = \frac{\rho_\infty ln(1 + B_M)}{M_{W,v}(C_{v,S} - C_{v,\infty})}\left[2.0 + \beta_c Re^{\frac{1}{2}} Sc^{\frac{1}{3}}\right]$$

$$B_M = \frac{Y_{v,S} - Y_{v,\infty}}{1 - Y_{v,S}}$$

Asymptotic models

The asymptotic models may be used when the asymptotic conditions are well satisfied.

At low Pe (Peclet number) limit:

$$Nu = 2\left[1 + \frac{1}{4}Pe + \frac{1}{8}Pe^2 \ln(Pe) + 0.01702Pe^2 + \frac{1}{32}Pe^3 \ln(Pe) + O(Pe^3)\right]$$

At high Pe limit:

$$Nu = 0.991Pe^{\frac{1}{3}}\left[1 + \frac{1}{16}Re + \frac{3}{160}Re^2 \ln(Re) + O(Re^2)\right]$$

Consideration of droplet interactions

- The model with consideration of droplet interactions is recommended when the spacing amongst droplets is not large enough.
- The effect of droplet interactions is more important when there is no forced convection or the forced convection is not strong.
- There is a proposed correction factor to take account of the interaction effect:

$$\eta_A = 1 - \frac{1}{1 + 0.725671\xi^{0.971716}} \qquad \xi = \frac{\left[\frac{4\pi V_A N}{3V_l}\right]^{1/3}}{[N^{1/3} - 1]N^{0.72}}$$

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