Modeling and Simulation of Water Evaporation from a Droplet of Polyvinylpyrrolidone (PVP) Aqueous Solution

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Abstract
This paper presents a model to describe the evaporation and drying behavior of a single spherical bi-component droplet containing evaporating liquid and dissolved solid substance. Although, many models are available in literature for droplet evaporation and drying, no appropriate model is available to study the liquid evaporation of a polymer aqueous solution. The present study concerns the evaporation and drying of a droplet of polymer (Polyvinylpyrrolidone - PVP) in the solvent water. The water evaporation rate from the droplet is computed using a modification of Abramzon and Sirignano’s model [1], to account for resistance from solid layer at the droplet surface. The effect of PVP presence on vapor pressure of water is estimated by calculating the activity coefficient of water using the UNIFAC-vdW-FV method [2]. The system under consideration is governed by the continuity (diffusion) and energy equations, which are solved using a finite difference method.

Figure 1 shows the temporal evolution of PVP mass fraction inside the droplet of initial size 200 µm at 20°C when subjected to hot nitrogen gas flowing at 1 m/s with temperature of 75°C. The droplet size recedes with time and the solute concentration builds up at the surface, which becomes more significant at the higher gas temperature. The influence of drying conditions such as relative humidity in the gas and gas velocity on evaporation and drying rate are also studied. The effect of relative humidity of 5% in the surrounding gas on droplet evaporation and drying is shown in Fig. 2 at the same condition. The times of 4 s (black lines) and 8 s (gray lines) are displayed. The no humidity condition (solid lines) is also shown for purpose of comparison. The PVP mass fraction is lower for higher relative humidity, whereas the water mass fraction is higher due to the smaller driving force for the mass transfer, delaying water evaporation. The differences between no humidity and 5% humidity situations build up with time: at 4 s, the droplet interior is hardly affected, and humidity starts influencing the outer region inside the droplet. At a later time, t = 8 s, the differences are large in the droplet core, and they are reduced towards the droplet surface, where the saturation solubility is reached. The study shows the UNIFAC-vdW-FV method to greatly improve the results of the UNIFAC model.

Droplet humidity, and both gas velocity and temperature strongly affect PVP/water droplet drying characteristics. The present model effectively captures the initial stages of single droplet drying. A more detailed knowledge of saturation solubility, the vapor diffusivity into the solid layer and its thermal conductivity is desirable.

Figure 1. Time evolution of PVP mass fraction inside the droplet
Figure 2. Effect of relative humidity (R.H.) on PVP mass fraction inside the droplet


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