



# Numerical simulation of evaporation and drying of a bi-component droplet



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## ABSTRACT

A mathematical model to describe the evaporation and drying behavior of a single quiescent spherical bi-component droplet containing evaporating liquid and dissolved solid substance is developed with primary focus on the application of this model to study the evaporation and drying of a droplet of polymer (Polyvinylpyrrolidone – PVP) in water and Mannitol in water. The water evaporation rate is computed using a convective two-film model with modifications to account for solid layer formation. The non-ideality effect induced by the presence of PVP or Mannitol on vapor pressure of water is accounted through the calculation of activity coefficient of water in either system. The problem under consideration is governed by the continuity (diffusion) and energy equations, which are solved using a finite difference method. The effect of drying conditions such as gas velocity, temperature, and relative humidity on evaporation and drying rate is studied. It is concluded that the present model effectively captures the initial stages of single droplet drying.

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## 1. Introduction

Spray drying is the widely used manufacturing technique in which the aerosol phase is dried to yield particles. The kinetics of the spray drying process is dominated by the moisture and temperature history of individual droplets. Even though the study of single droplet evaporation and drying does not take into account many of the complex interactions as in spray drying, it offers a practical method to gain insight into the evaporation and drying process as well as particle characteristics at individual particle level. Single droplet evaporation and drying constitutes the basis for any spray drying process.

Many studies present the evaporation phenomena associated with pure and multi-component droplet, but there is a lack of a mathematical model which can predict the evaporation and drying behavior of a droplet containing a polymer or sugar dissolved in water because of the unknown physical behavior, unavailability of experimental results and complexity of the problem. Charlesworth and Marshall [5] first investigated the concept of single droplet evaporation and drying by measuring the change in droplet mass using the deflection of a thin, long glass filament. This study [5] also classifies different stages of droplet evaporation. Later, this experiment with some modifications is considered in many studies. The work of Sano and Keey [29] includes the drying behavior

of colloidal material into a hollow sphere by considering the migration of solid matter towards the center of the droplet through the convection measurement inside the droplet, which is a challenge to experiment [28]. Most of the experiments concerning the droplet evaporation and drying available in literature are either related to salts [5,3,30], milk powders [6,13] or some other colloidal matter [29,28,27,17], but none deal with droplets of polymer or Mannitol as a constituent. Previously developed models assume a uniform temperature gradient within the droplet [28,3,27] and neglect the effect of solid formation [3,13,27]. The study of Nestic and Vodnik [28] presents the kinetics of droplet evaporation to predict the drying characteristics of a colloidal silica droplet, where the crust formation on the surface occurring in this configuration is considered. The surface vapor concentration of evaporating solvent is calculated using experimental material dependent factors, which are not available for every solution including polymer and Mannitol solutions in water. Moreover, in case of a polymer, molecular entanglement leads to solid layer formation. Nestic and Vodnik [28] use a more detailed description of various stages of droplet evaporation and drying. These stages include the initial rise of droplet temperature to an equilibrium value and continuous solvent evaporation causing an increase of the solute mass fraction within the droplet. When the solute mass fraction at the droplet surface rises to a critical value, a thin solid layer forms, and further drying leads to a dried particle. Farid [13] shows that the droplet evaporation and drying are controlled by thermal-diffusion rather than mass-diffusion as assumed by most of the earlier studies [5,29,3]. In Farid's model [13], the time taken for the formation

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of crust on a colloidal silica droplet is calculated using the energy balance, which does not account for solvent and solute composition changes, and the evaporation rate is computed using a simple relation without accounting for the variation in film and liquid properties. For droplets with suspended solids inside, the population balance approach is recently developed [17] to model the nucleation and growth of suspended solids inside an ideal binary liquid droplet with an assumption that there exist some nuclei of suspended solids initially, but this method cannot be applied in the present case of droplet with polymers, as solute is completely dissolved in water. Golman et al. [15] present a model for the evaporation and drying of slurry droplets, which is an improvement over the receding interface model of Cheong et al. [7] for slurry droplets, but in this study [15], the bi-component liquid mixture is treated as ideal. A detailed review of all existing theoretical models of evaporation and drying of single droplet containing dissolved and insoluble solids is given by Mezhericher et al. [26].

The aim of the present work is to develop a mathematical model, which can be applied to predict the evaporation and drying characteristics of droplets of the polymer PVP (Polyvinylpyrrolidone) and for Mannitol dissolved in water solutions. Prerequisites of the method are accounting for the solid layer resistance in mass evaporation rate and energy calculation, and treatment of the liquid mixture as non-ideal by computing the activity coefficient of the evaporating component.

## 2. Mathematical model

### 2.1. Problem description

The problem under consideration is the evaporation and drying of an isolated single spherical droplet consisting of a binary mixture of a liquid and a dissolved solid material with low or zero vapor pressure.

During the evaporation and drying of the bi-component droplet, the droplet undergoes four stages as explained by Nescic and Vodnik [28], see Fig. 1. In the initial stage, the droplet temperature quickly rises to an equilibrium temperature, which is most often near to the wet bulb temperature for surrounding gas and humidity, with some solvent evaporation.

In the second stage, the droplet starts to shrink as solvent evaporates and solute mass fraction increases at the surface; this leads to slight raise in the droplet temperature. The increase in solute mass fraction at the droplet surface hinders further evaporation as vapor pressure of the solvent at the surface drops. The third stage of drying starts when the solute mass fraction at the surface raises to a threshold value, which most often is equal to the saturation solubility of the solute in the solvent, whereupon the crust formation starts for salts, sugar and colloidal material and in the case of polymers, molecular entanglement and gradual increase

in concentration lead to solid layer formation at the droplet surface. In the latter case, the solid layer thickens and develops into the droplet interior as depicted in Fig. 1, and a rapid fall in evaporation rate is observed. In this period, the heat penetrated into the liquid is used for heating the droplet causing the droplet temperature to rise rapidly. Further drying behavior of droplet depends on the vapor diffusivity through the solid layer. In the final stage of drying, boiling followed by particle drying, eventually leading to dried product formation, takes place.

In the next section, the general mathematical formulation for an evaporating and drying droplet is presented with the primary focus on the drying behavior of a PVP in water and Mannitol in water droplet. The numerical method, results and discussion are presented thereafter.

### 2.2. Mathematical formulation

The problem of evaporation and drying of single droplet can be well defined using the diffusion and heat conduction equations in spherical coordinates. The diffusion equation for the substance  $i$  in the droplet is formulated in terms of mass fraction  $Y_i$ , reads

$$\frac{\partial Y_i}{\partial t} = \frac{D_{12}}{r^2} \left[ \frac{\partial}{\partial r} \left( r^2 \frac{\partial Y_i}{\partial r} \right) \right], \quad (1)$$

where  $D_{12}$  is the binary diffusion coefficient in the liquid,  $r$  is the radial coordinate, and  $t$  stands for time. In this equation,  $i = 1$  denotes the solvent (water) and  $i = 2$  denotes solute (PVP or Mannitol). Initially, the droplet is a homogenous mixture,  $Y_i = Y_{i0}$  at  $t = 0$  s. At the droplet center,  $r = 0$  m, the regularity condition must be satisfied at any time,  $\partial Y_i / \partial r = 0$ . The boundary condition at the droplet surface must account for the change in droplet size,

$$-D_{12} \frac{\partial Y_i}{\partial r} - Y_i \frac{\partial R}{\partial t} = \frac{\dot{m}_i}{A \rho_l} \quad (2)$$

at  $r = R(t)$ . Here  $\dot{m}$  is the mass evaporation rate of substance  $i$  across the droplet surface,  $R(t)$  and  $A(t)$  are time dependent droplet radius and surface area, respectively, and  $\rho_l$  is the liquid density.  $\dot{m}$  is zero for non-evaporating solute (PVP or Mannitol),  $i = 2$ . The diffusion process described through Eq. (1) provides the mass fraction profiles inside the droplet. For solving this equation, the evaporation rate from the droplet surface,  $\dot{m}$  is needed, which appears in Eq. (2). This rate of evaporation is determined based on Sherwood analogy of Abramzon and Sirignano's model [1], and in the present study, it is used in the extended form for a bi-component liquid mixture as modified by Brenn et al. [4],

$$\dot{m} = \sum_{i=1}^N 2\pi R_i \rho_{i,f} D_{i,f} \widetilde{Sh} \ln(1 + B_{M,i}), \quad (3)$$

where  $R_i$  is volume equivalent partial radius of component  $i$ , based on its corresponding volume fraction, computed as  $R_i = R(V_i/V)^{1/3}$ ,  $\widetilde{Sh}$  is the modified Sherwood number, which accounts for the effect of convective droplet evaporation [1],  $D_{i,f}$  is vapor diffusivity of component  $i$ , and  $\rho_{i,f}$  is density of component  $i$  in the film.  $B_{M,i}$  is the Spalding mass transfer number for component  $i$ , and it is calculated as [1,20],

$$B_{M,i} = \frac{Y_{i,s} - Y_{i,\infty}}{1 - Y_{i,s}}, \quad (4)$$

where  $Y_{i,s}$  and  $Y_{i,\infty}$  are the mass fractions of evaporating component  $i$  at the droplet surface and in the bulk of the gas, respectively. Nescic and Vodnik [28] implemented a similar approach, but they do not account for the volume fraction based radius in the calculation of the evaporation rate, i.e., droplet radius  $R$  is used instead of  $R_i$  in computing  $\dot{m}$ . Since the solute vapor pressure is low or zero and the droplet's solute evaporation rate is zero or very small, negli-

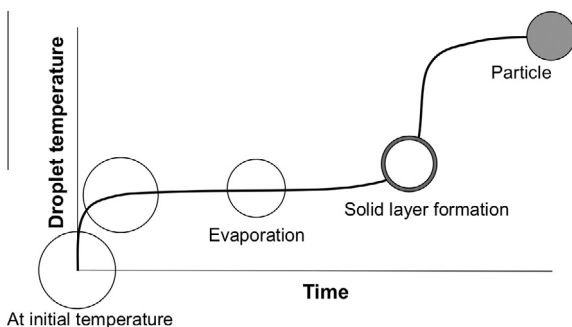


Fig. 1. Schematic diagram of stages in single droplet evaporation and drying.

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