An analytical solution to the spherically symmetric species diffusion equation: application to modelling of heating and evaporation of bi-component droplets

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Abstract

An analytical solution to the spherically symmetric species diffusion equation is suggested. This solution includes an additional term, exponentially increasing with time, in the series. This term does not lead to an unphysical result due to the fact that the solution of the species mass diffusion equation is valid for mass fractions in the range from 0 to 1. This imposes the restriction on the range of its validity. Based on this solution, a simplified model for bi-component droplet heating and evaporation is developed and applied to the analysis of the observed average temperature of droplets in a monodisperse spray. The model takes into account all key processes, which take place during droplet heating and evaporation, including the distribution of temperature and the diffusion of liquid species inside the droplet and the effects of the non-unity activity coefficient (ideal and non-ideal models). The predicted time evolution of the average temperatures is shown to be reasonably close to the measured ones, especially in the case of pure ethanol and 50% ethanol – 50% acetone mixture droplets. The temperatures predicted by the ideal and non-ideal models differ by not more than several degrees. The predicted radial distributions of temperature and species mass fractions inside droplets are consistent with the physical nature of the process under consideration. The non-zero gradient of the mass fraction of ethanol inside the droplet shows the limitations of widely-used models, based on the assumptions of either zero or infinitely large species diffusivities inside droplets.

Introduction

In [1] a model for the heating and evaporation of monocomponent droplets, based on the analytical solution of the heat conduction equation inside droplets, was suggested. The practical application of this model, however, is limited by the fact that most real-life fuels are multi-component. The models of multi-component droplet heating and evaporation could be subdivided into two main groups: those based on the analysis of individual components [2], applicable in the case when a small number of components needs to be taken into account, and those based on the probabilistic analysis of a large number of components (see review [3]). In the second family of models a number of additional simplifying assumptions were used, including the assumption that species inside droplets mix infinitely quickly. The focus of this paper is on the extension of the model, developed in [1] for monocomponent droplets, to the case of multi-component droplets. Only the first group of multi-component droplet heating and evaporation models is considered, which allows us to perform the deterministic analysis of individual species. Moreover, at this stage only the simplest case of bi-component droplets is considered, as in [2], which allows us to get a better understanding of the underlying physics of the processes involved. The new model is based on the analytical solution of the spherically symmetric species diffusion equation, which has not yet been reported to the best of our knowledge. It is much simpler than the previously suggested models (e.g. [2]) which makes it potentially attractive for implementation into computational fluid dynamics (CFD) codes. The predictions of the model are compared with the measured time evolution of droplet temperatures in monodisperse bi-component (ethanol/acetone) droplet streams.

The species diffusion equation for spherically symmetric droplets

Assuming that the processes inside droplets are spherically symmetric (no convection), equations for mass fractions of liquid species $Y_{li} \equiv Y_{li}(t, R)$ inside them can be presented in the following form:

$$\frac{\partial Y_{li}}{\partial t} = D_l \left(\frac{\partial^2 Y_{li}}{\partial R^2} + \frac{2}{R} \frac{\partial Y_{li}}{\partial R} \right), \tag{1}$$

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where $i = 1, 2$, D_l is the liquid mass diffusivity. Equations (1) are solved with the following boundary conditions:

$$\alpha(\epsilon_i - Y_{lis}) = -D_l \left.\frac{\partial Y_{li}}{\partial R}\right|_{R=R_d-0}, \tag{2}$$

and the initial conditions $Y_{li}(t = 0) = Y_{li0}(R)$, where $Y_{lis} = Y_{lis}(t)$ are liquid components mass fractions at the droplet's surface, $\alpha = |\dot{m}_d|/(4\pi\rho_l R_d^2)$, $\dot{m}_d$ is the droplet evaporation rate. We are interested only in a solution which is continuously differentiable twice in the whole domain. This implies that Y_{li} should be bounded for $0 \leq R < R_d$. Moreover, the physical meaning of Y_{li}, as the mass fraction, implies that $0 \leq Y_{li} \leq 1$.

Although Equations (1) with boundary conditions (1) look similar to the equation considered in [1], the solution suggested in [1] cannot be used for the above problem. The new analytical solution to this equation, subject to above boundary and initial conditions, was obtained. This solution was incorporated into a zero dimensional code used for modelling the heating and evaporation of bi-component droplets, along with a number of other models, taking into account the distribution of temperature inside the droplet and the effects of the non-unity activity coefficient (ideal and non-ideal models). The effects of recirculation in the moving droplets on heat and mass diffusion are taken into account using the effective thermal conductivity and the effective diffusivity models. The predictions of this zero-dimensional code were compared with experimental results reported in [2].

Results and Discussion

The comparison between the predictions of the model and experimental data has shown that the model underpredicts the average droplet temperature at the final stages of droplet heating and evaporation in the case of pure acetone and acetone rich droplets. There is a general agreement between the predicted and observed average temperatures in the case of pure ethanol and 50% ethanol – 50% acetone mixture droplets. In the case of 75% ethanol – 25% acetone mixture droplets, the predicted average droplet temperature was several degrees higher than the observed one. It was shown that the temperatures predicted by the simplified model and the earlier reported vortex model were reasonably close. Also, the temperatures predicted by the ideal and non-ideal models differ by not more that several degrees. The application of the simplified model with the activity coefficient equal to 1 to the interpretation of the time evolution of temperatures measured with similar errors can therefore be justified. The predicted radial distributions of temperature and species mass fractions inside droplets are consistent with the physical nature of the phenomenon.

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Nomenclature

D	diffusion coefficient [m^2/ s]
m	mass [kg]
R	distance from the droplet centre [m]
Y	mass fraction
ϵ	evaporation rate of species
ρ	density [kg·s^{-3}]

Subscripts

d	droplet
i	species
l	liquid

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