A model for a bi-component droplet heating and evaporation

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Introduction

- For a single component droplet, there is only heat diffusion in the liquid phase and there are heat and mass diffusion in the gas phase.

- For a bi-component droplet, there are heat and mass diffusion in both liquid and gas phases.

Heat diffusion in the liquid phase

- Heat conduction equation inside the droplet:

$$\frac{\partial T}{\partial t} = \kappa \left(\frac{\partial^2 T}{\partial R^2} + \frac{2}{R} \frac{\partial T}{\partial R} \right)$$

- Boundary conditions without evaporation:

$$h(T_g - T_s) = k_l \left. \frac{\partial T}{\partial R} \right|_{R=R_d-0},$$

$$\left. \frac{\partial T}{\partial R} \right|_{R=0} = 0,$$

Heat diffusion in the liquid phase

- The solution of the heat conduction equation without evaporation for *h* = const is presented as follows:

$$T(R,t) = \frac{R_d}{R}\sum_{n=1}^{\infty}\left\{q_n \exp\left[-\kappa_R\lambda_n^2 t\right] - \frac{\sin\lambda_n}{\|v_n\|^2\lambda_n^2}\mu_0(0)\exp\left[-\kappa_R\lambda_n^2 t\right] - \right.$$

$$\left. - \frac{\sin\lambda_n}{\|v_n\|^2\lambda_n^2}\int_0^t \frac{\mathrm{d}\mu_0(\tau)}{\mathrm{d}\tau}\exp\left[-\kappa_R\lambda_n^2(t-\tau)\right]\mathrm{d}\tau\right\}\sin\left[\lambda_n\left(\frac{R}{R_d}\right)\right] + T_g(t),$$

Heat diffusion in the liquid phase

- λ_n are the solutions of the equation:

$$\lambda \cos \lambda + h_0 \sin \lambda = 0,$$

$$|| v_n ||^2 = \frac{1}{2}\left(1 - \frac{\sin 2\lambda_n}{2\lambda_n}\right) = \frac{1}{2}\left(1 + \frac{h_0}{h_0^2 + \lambda_n^2}\right),$$

$$q_n = \frac{1}{R_d || v_n ||^2} \int_0^{R_d} \tilde{T}_0(R) \sin\left[\lambda_n \left(\frac{R}{R_d}\right)\right] \mathrm{d}R,$$

$$\kappa_R = \frac{k_l}{c_l \rho_l R_d^2}, \qquad \mu_0(t) = \frac{h T_g(t) R_d}{k_l},$$

- h_0 $\quad h_0 = (hR_d/k_l) - 1$

Heat diffusion in the liquid phase

- The effect of droplet evaporation has been taken into account by replacing gas temperature by the so-called effective temperature.

$$T_{\text{eff}} = T_g + \frac{\rho_l L \dot{R}_d}{h}$$

Mass diffusion in the liquid phase

- Mass fraction equation inside the droplet:

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

- Boundary conditions:

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

$$\left. \frac{\partial Y_{li}}{\partial R} \right|_{R=0} = 0$$

- where $\alpha_i = \frac{D_g \rho_{\mathrm{total}} \ln(1 + B_M)}{\rho_l R_d}$

Mass diffusion in the liquid phase

- The solution of the mass fraction equation for $\alpha_i = \mathrm{const}$ is presented as follows:

$$Y_{li}(R,t) = \frac{R_d}{R} \sum_{n=1}^{\infty} \left\{ q_n \exp\left[-\kappa_R \lambda_n^2 t\right] - \frac{\sin\lambda_n}{\| v_n \|^2 \lambda_n^2} \mu_0(0) \exp\left[-\kappa_R \lambda_n^2 t\right] - \right.$$

$$\left. - \frac{\sin\lambda_n}{\| v_n \|^2 \lambda_n^2} \int_0^t \frac{\mathrm{d}\mu_0(\tau)}{\mathrm{d}\tau} \exp\left[-\kappa_R \lambda_n^2 (t-\tau)\right] \mathrm{d}\tau \right\} \sin\left[\lambda_n \left(\frac{R}{R_d}\right)\right] + \epsilon_i(t),$$

Mass diffusion in the liquid phase

- λ_n are the solutions of the equation:

$$\lambda \cos\lambda + h_0 \sin\lambda = 0,$$

$$\| v_n \|^2 = \frac{1}{2}\left(1 - \frac{\sin 2\lambda_n}{2\lambda_n}\right) = \frac{1}{2}\left(1 + \frac{h_0}{h_0^2 + \lambda_n^2}\right),$$

$$q_n = \frac{1}{R_d \| v_n \|^2} \int_0^{R_d} \tilde{Y}_{li0}(R) \sin\left[\lambda_n \left(\frac{R}{R_d}\right)\right] \mathrm{d}R,$$

$$\kappa_R = \frac{D_l}{R_d^2}, \qquad \mu_0(t) = -\frac{\alpha_i \epsilon_i(t) R_d}{D_l},$$

- $h_0 = (-\alpha_i R_d / D_l) - 1$ and $\epsilon_i = \dfrac{Y_{vis}}{\sum_i Y_{vis}},$

Heat and mass transfer

- The total evaporation rate of the droplet:

$$\dot{m} = \pi \rho_{\mathrm{ref}} D D_i B_{\mathrm{M},i} Sh_i$$

- Heat transfer coefficient (*h*) is calculated using Nusselt number equation (Nu):

$$\mathrm{Nu} = 2R_d h / k_g$$

Heat and mass transfer

- Nusselt number

$$Nu_{\mathrm{iso}} = \frac{\ln(1+B_{\mathrm{T}})}{B_{\mathrm{T}}}\left(2 + \frac{0.6Re^{1/2}\mathrm{Pr}^{1/3}}{F(B_{\mathrm{T}})}\right)$$

- Sherwood number

$$Sh_{i,\mathrm{iso}} = \frac{\ln(1+B_{\mathrm{M},i})}{B_{\mathrm{M},i}}\left(2 + \frac{0.6Re^{1/2}Sc_i^{1/3}}{F(B_{\mathrm{M},i})}\right)$$

Heat and mass transfer

- The effect of interacting between droplets was taken into account using the following equation :

$$\eta(C) = \frac{Nu}{Nu_{iso}} = \frac{Sh}{Sh_{iso}}$$

- where C is the distance parameter (distance between droplets divided by their diameters)

$$\eta(C) = 1 - 0.57\left(1 - \frac{1 - 0.57e^{-0.13(C-6)}}{1 + 0.57e^{-0.13(C-6)}}\right)$$

Species mass fractions at the droplet surface

- Knowing the liquid mass fraction at droplet surface Y_{li} as initial value or from the solution of species diffusion equation then we can calculate the following:

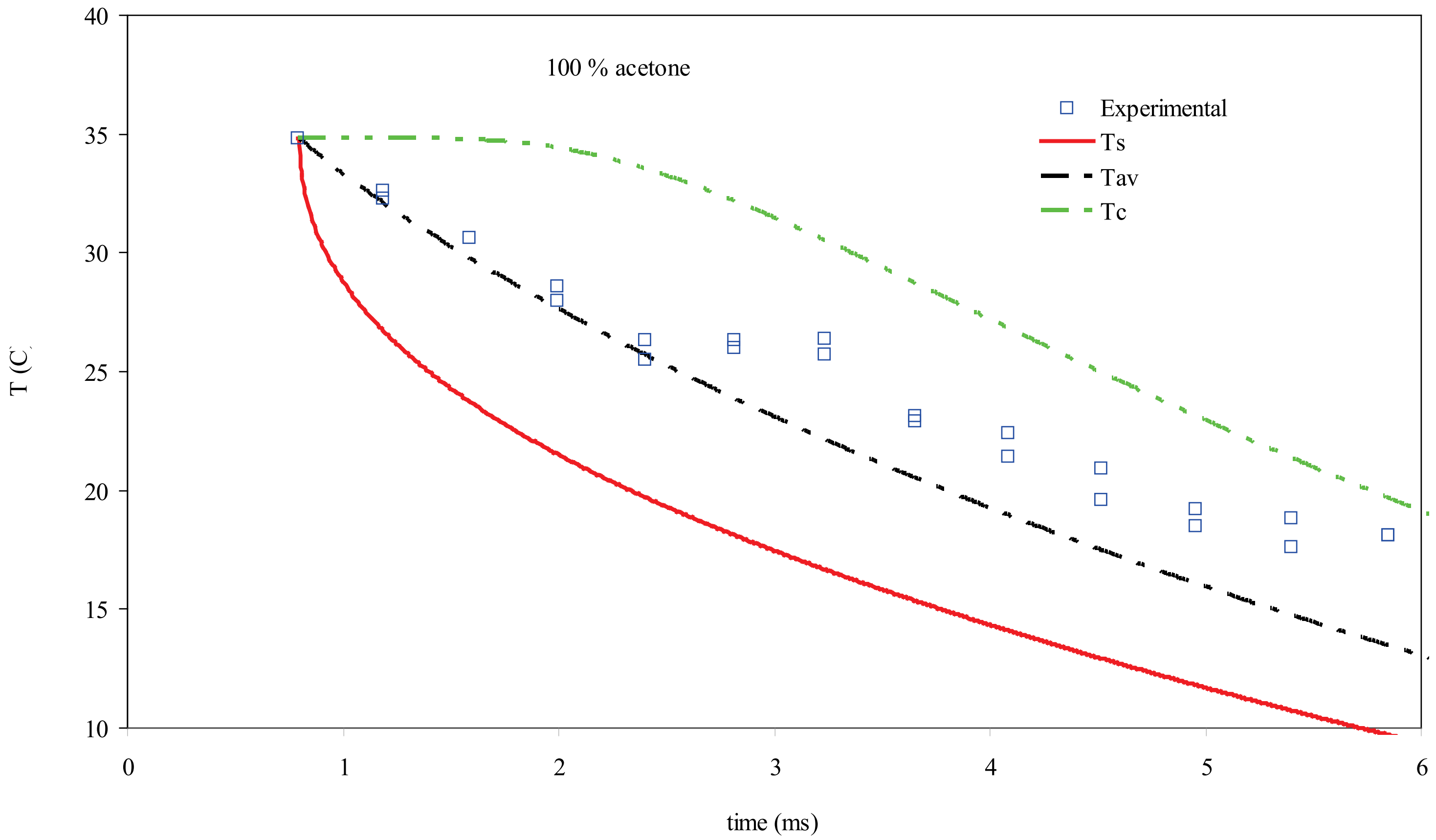
$$\chi_{li} = \frac{Y_{li}/M_i}{\sum_i (Y_{li}/M_i)}$$

$$\chi_{i,g,S} P_a = \chi_{i,l,S} \gamma_i P_{sat}(T_S)$$

- where γ_i is the activity coefficient and as a first step we put it equal to 1 (ideal mixture).

$$Y_{vi} = \frac{\chi_{vi} M_i}{\sum_i (\chi_{vi} M_i) + \chi_{\text{air}} M_{\text{air}}}$$

Preliminary results



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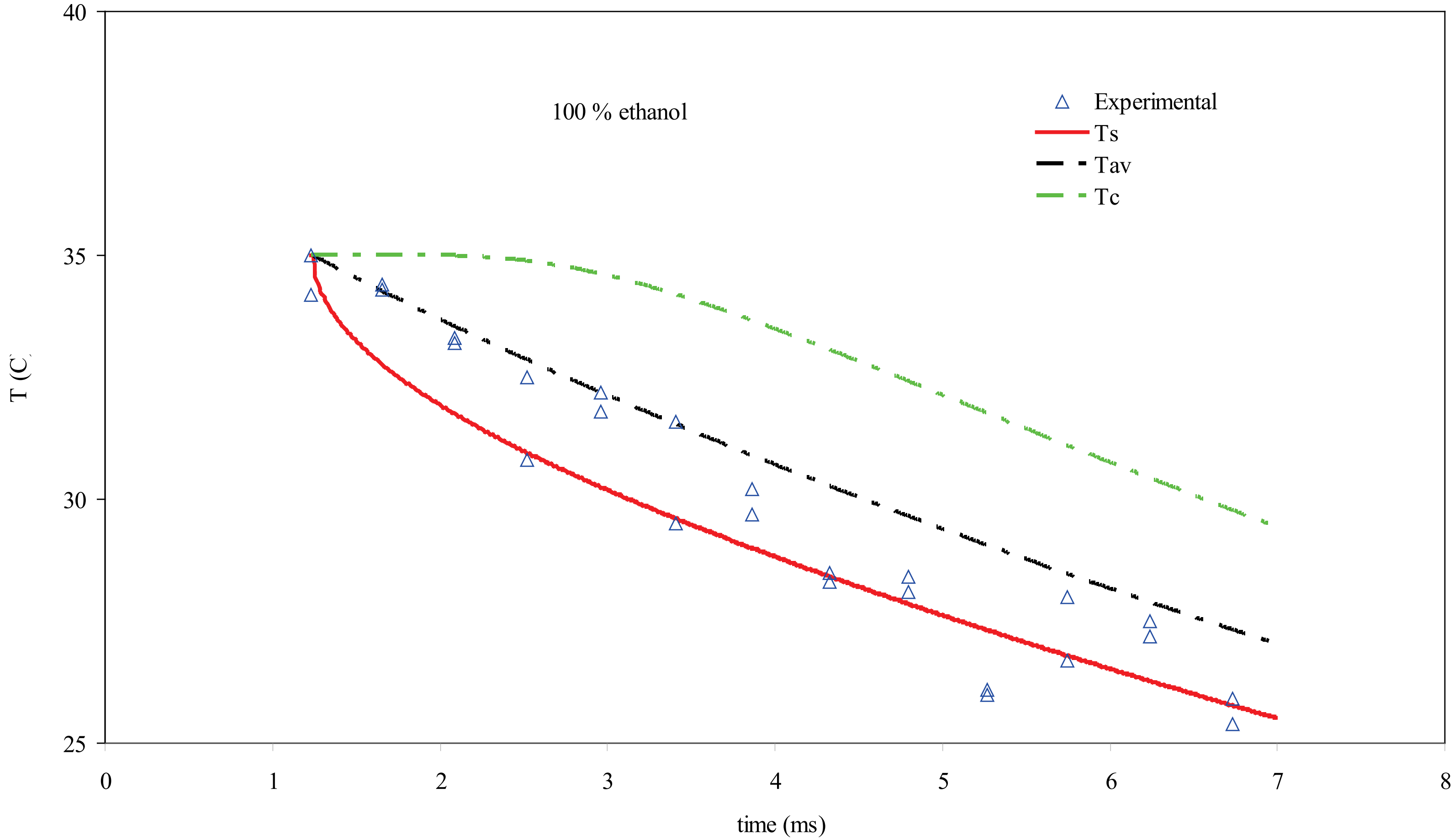

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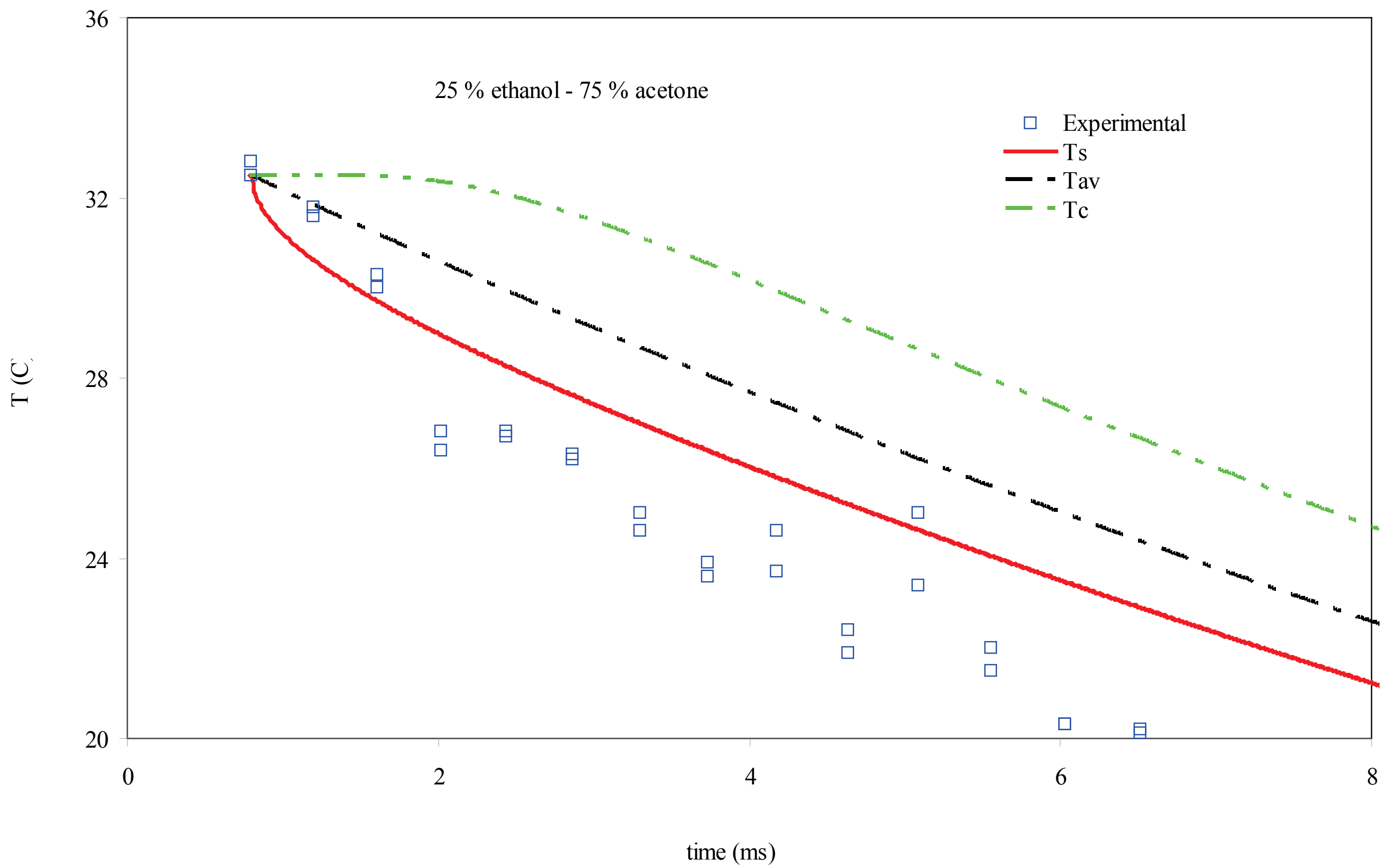

Thank you for your attention

Your questions are more than welcome

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