Modelling of heating and evaporation of multi-component droplets, taking into account the diffusion of species

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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.
- As a first stage, we have ignored the effect of fuel vapour on the gas phase ‘’Oneway Solution’’ then we have taken it into account ‘’Coupled Solution’’

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 $h_0 = (hR_d/k_l) - 1$

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.

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

Species 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:

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

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

- where $\alpha = \frac{|\dot{m}_d|}{4\pi \rho_l R_d^2}$

Species diffusion in the liquid phase

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

$$Y_{li} = \epsilon_i + \frac{1}{R}\left\{\left[\exp\left[D_l\left(\frac{\lambda_0}{R_d}\right)^2 t\right]\left[q_{i0} - Q_0\left(\epsilon_i(0) + \frac{R_d^2}{D_l\lambda_0^2}\epsilon_i'\right)\right]\right.\right.$$
$$\left. + Q_0\frac{R_d^2}{D_l\lambda_0^2}\epsilon_i'\right]\sinh\left(\lambda_0\frac{R}{R_d}\right)$$
$$+\sum_{n=1}^{\infty}\left[\exp\left[-D_l\left(\frac{\lambda_n}{R_d}\right)^2 t\right]\left[q_{in} - Q_n\left(\epsilon_i(0) - \frac{R_d^2}{D_l\lambda_n^2}\epsilon_i'\right)\right]\right.$$
$$\left.\left. - Q_n\frac{R_d^2}{D_l\lambda_n^2}\epsilon_i'\right]\sin\left(\lambda_n\frac{R}{R_d}\right)\right\}.$$

$$Q_n = \begin{cases} -\frac{1}{||v_0||^2}\left(\frac{R_d}{\lambda_0}\right)^2(1+h_0)\sinh\lambda_0 & \text{when} \quad n=0 \\ \frac{1}{||v_n||^2}\left(\frac{R_d}{\lambda_n}\right)^2(1+h_0)\sin\lambda_n & \text{when} \quad n\geq 1 \end{cases}$$

Species diffusion in the liquid phase

- $$q_{in} = \frac{1}{||v_n||^2} \int_0^{R_d} R Y_{li0}(R) v_n(R) \mathrm{d}R$$
- λ_n are the solutions of the equation:

$$(\lambda \cos \lambda + h_0 \sin \lambda) = 0$$

$$||v_n||^2 = \int_0^{R_d} v_n^2(R) \mathrm{d}R = \frac{R_d}{2} \left[1 + \frac{h_0}{h_0^2 + \lambda_0^2} \right]$$

- λ_0 is the solution of $(\lambda \cosh \lambda + h_0 \sinh \lambda) = 0$

$$||v_0||^2 = \int_0^{R_d} v_0^2(R) \mathrm{d}R = -\frac{R_d}{2} \left[1 + \frac{h_0}{h_0^2 - \lambda_0^2} \right]$$

- $h_0 = -\left(1 + \frac{\alpha R_d}{D_l}\right)$ and $\epsilon_i = \frac{Y_{vis}}{\sum_i Y_{vis}}$

Heat and mass transfer

- The total evaporation rate of the droplet:

$$\dot{m}_d = -2\pi R_d D_v \rho_{\text{total}} B_M \text{Sh}_{\text{iso}}$$

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

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

Heat and mass transfer

- Nusselt number

$$\mathrm{Nu_{iso}} = 2\frac{\ln(1+B_T)}{B_T}\left(1+\frac{(1+\mathrm{Re}_d\mathrm{Pr}_d)^{1/3}\max\left[1,\mathrm{Re}_d^{0.077}\right]-1}{2F(B_T)}\right)$$

- Sherwood number

$$\mathrm{Sh_{iso}} = 2\frac{\ln(1+B_M)}{B_M}\left(1+\frac{(1+\mathrm{Re}_d\mathrm{Sc}_d)^{1/3}\max\left[1,\mathrm{Re}_d^{0.077}\right]-1}{2F(B_M)}\right)$$

Heat and mass transfer

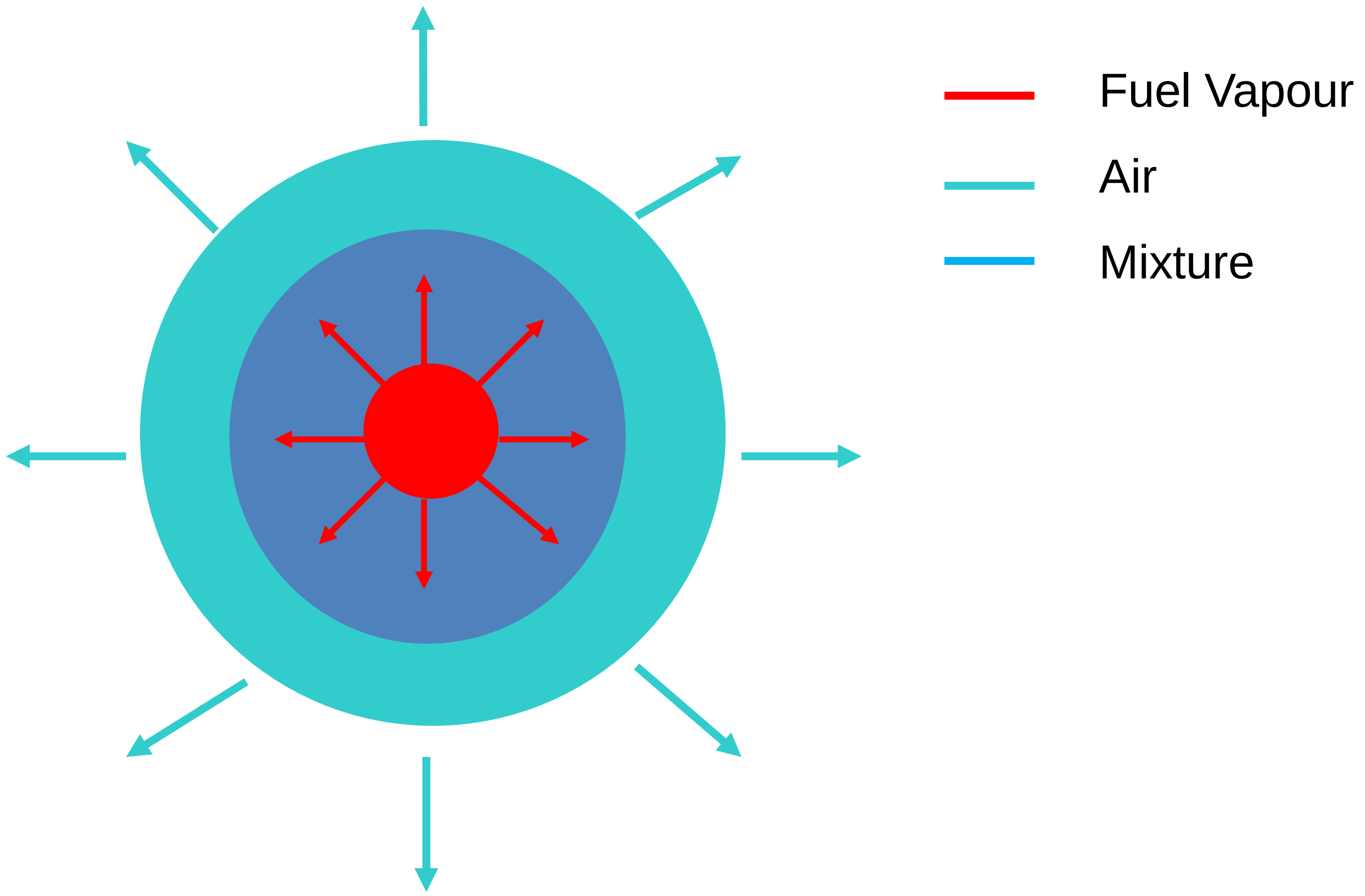
- The effect of interacting between droplets was taken into account using the following equation :

$$\eta(C) = \frac{\mathrm{Sh}}{\mathrm{Sh_{iso}}} = \frac{\mathrm{Nu}}{\mathrm{Nu_{iso}}} = 1 - 0.57\left(1 - \frac{1 - 0.57\exp\left[-0.13(C-6)\right]}{1 + 0.57\exp\left[-0.13(C-6)\right]}\right)$$

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

Coupled solution

The effect of fuel vapour on the gas phase properties will be taken into account.



Coupled solution

$$m_{air} = \rho_{air} \times Vol \qquad Vol = Vol_{cell} - Vol_{droplet} \qquad R_{cell} = \sqrt{(D_l \times t_{obs})}$$

where D_l is the liquid diffusivity, t_{obs} is the observation time = 10 ms and R_{cell} is the radius of the sphere of influence.

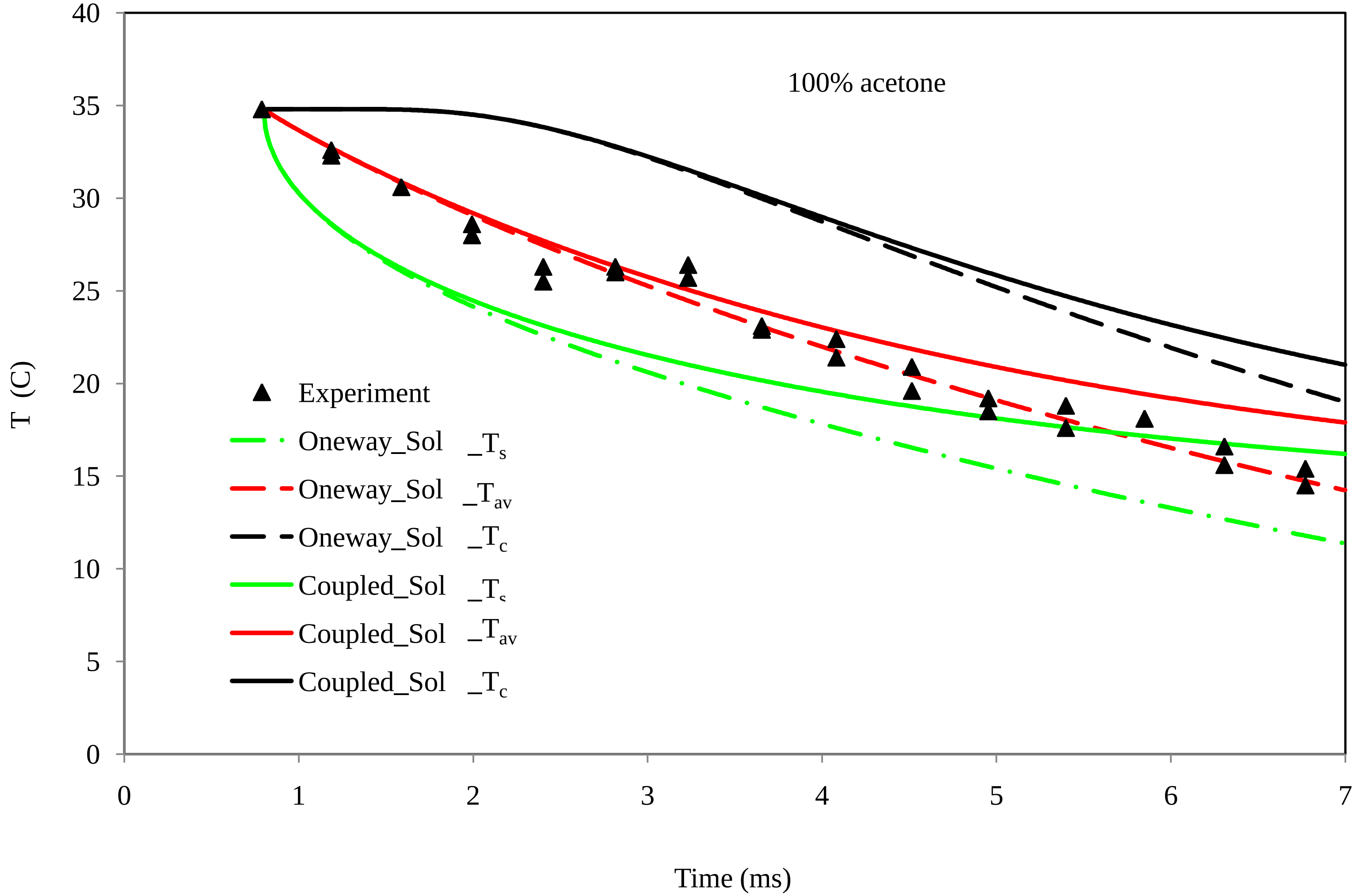
To calculate the new mass of air, We used the following equation:

$$m_{air} = N_{air} \times M_{air}$$

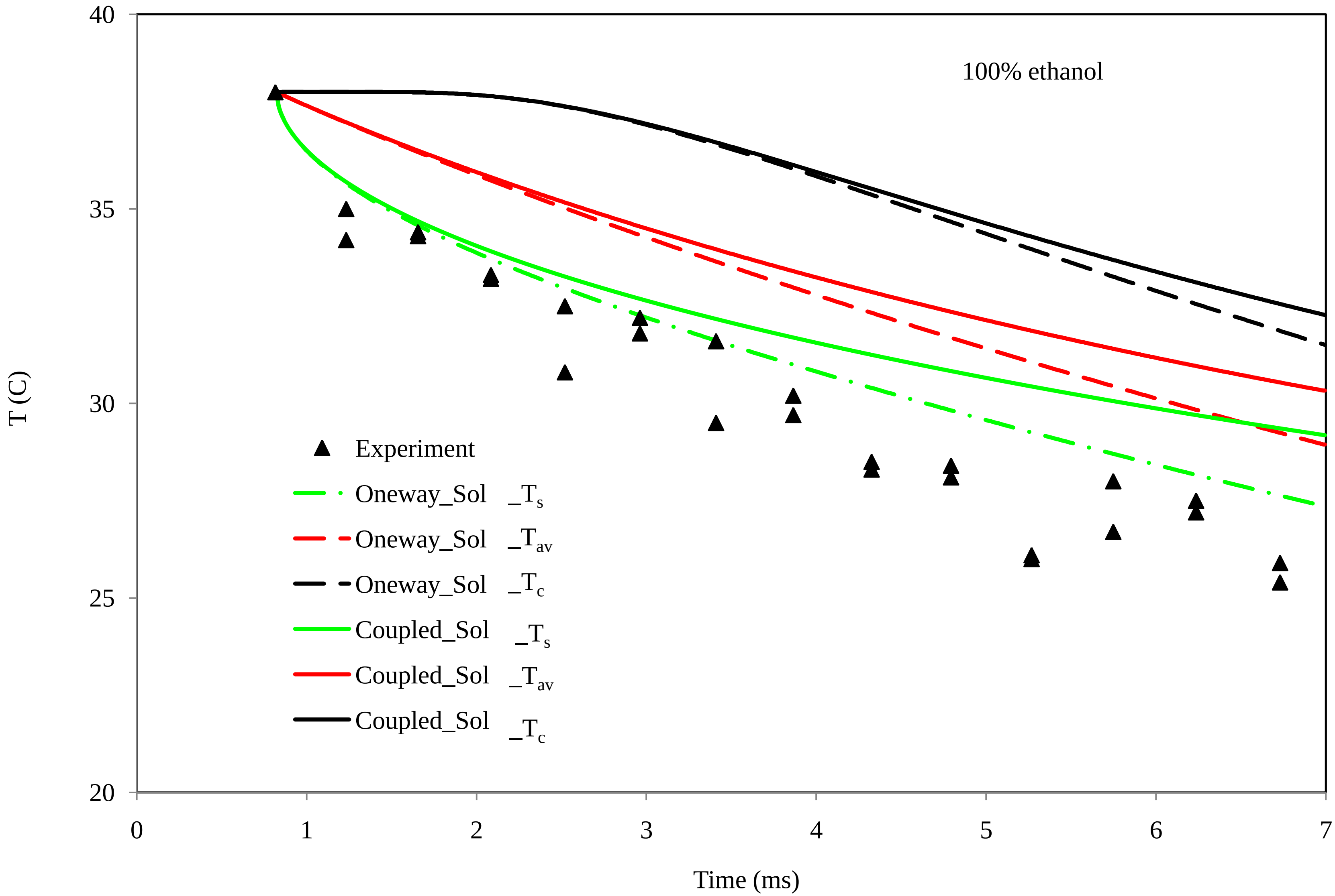
$$N_{air} = N_{air,initial} - N_{vapour}$$

$$N_{vapour} = N_{ethanol} + N_{acetone}$$

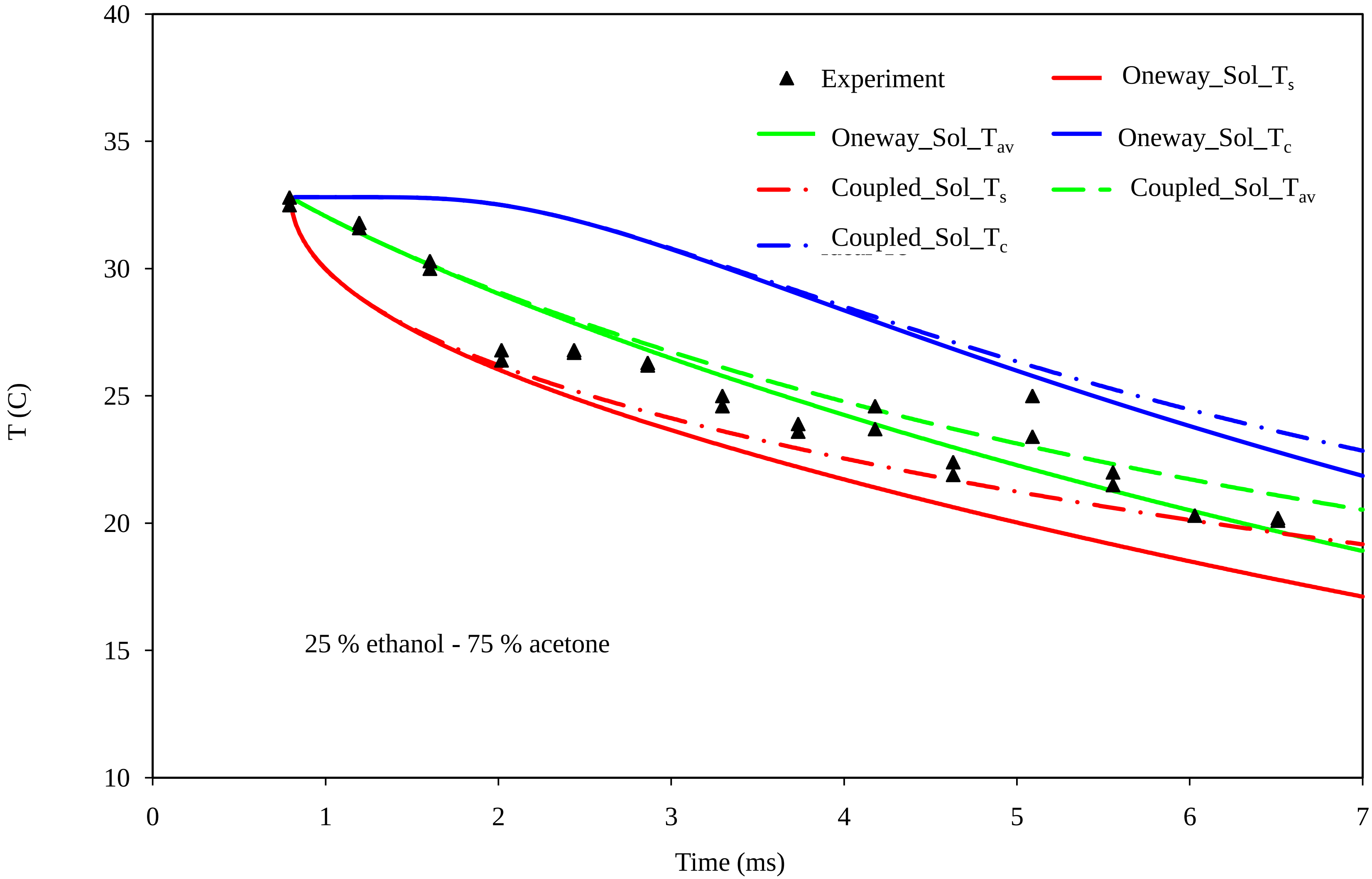
Results


100% acetone
T (C)
Time (ms)
0
5
10
15
20
25
30
35
40
0
1
2
3
4
5
6
7
Experiment
Oneway_Sol _Ts
Oneway_Sol _Tav
Oneway_Sol _Tc
Coupled_Sol _Ts
Coupled_Sol _Tav
Coupled_Sol _Tc

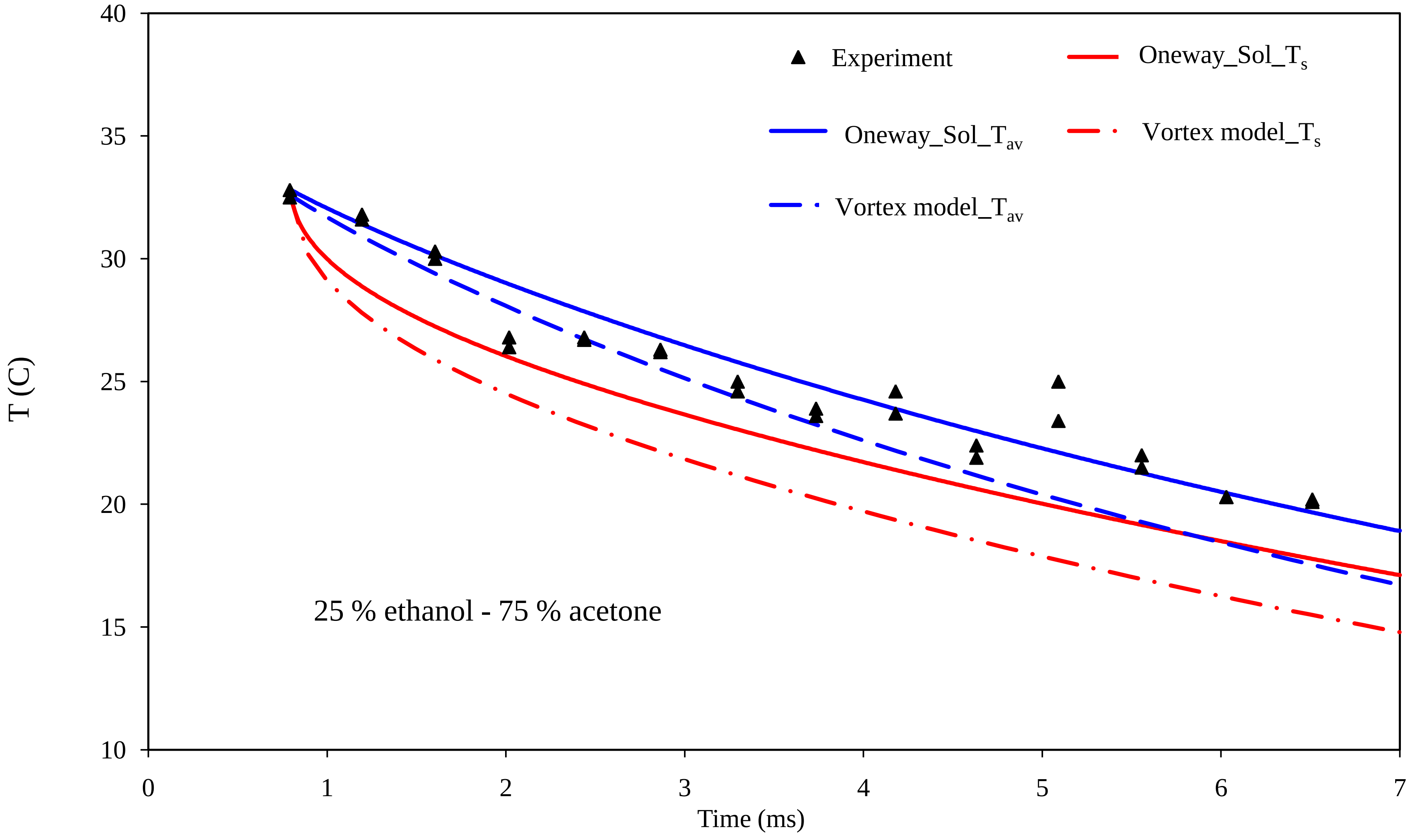
Results


40
35
30
25
20
T (C)
0
1
2
3
4
5
6
7
Time (ms)
100% ethanol
Experiment
Oneway_Sol _Ts
Oneway_Sol _Tav
Oneway_Sol _Tc
Coupled_Sol _Ts
Coupled_Sol _Tav
Coupled_Sol _Tc

Results

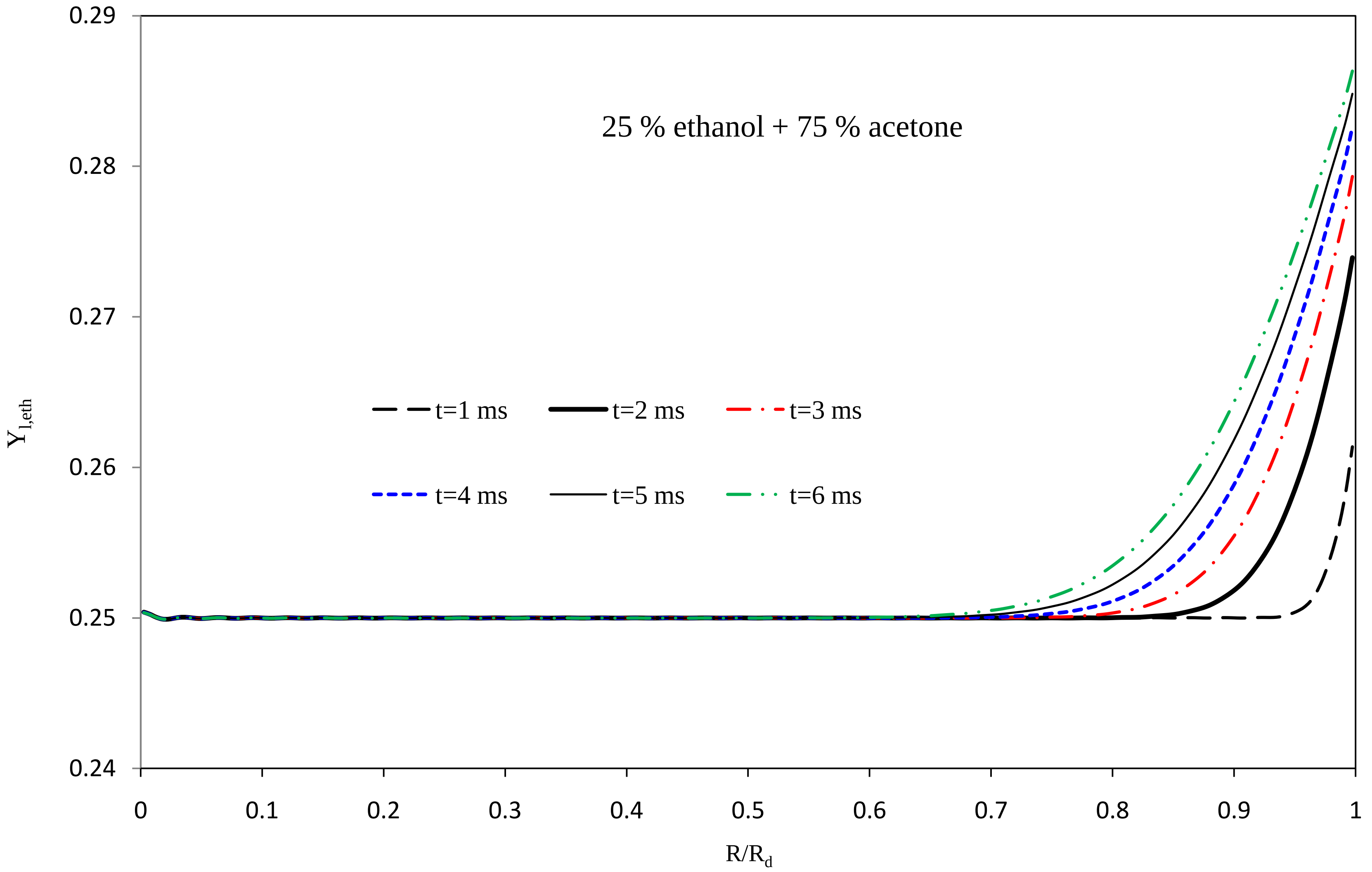

Experiment
Oneway_Sol_Ts
Oneway_Sol_Tav
Oneway_Sol_Tc
Coupled_Sol_Ts
Coupled_Sol_Tav
Coupled_Sol_Tc
25 % ethanol - 75 % acetone
T (C)
Time (ms)
40
35
30
25
20
15
10
0
1
2
3
4
5
6
7

Results

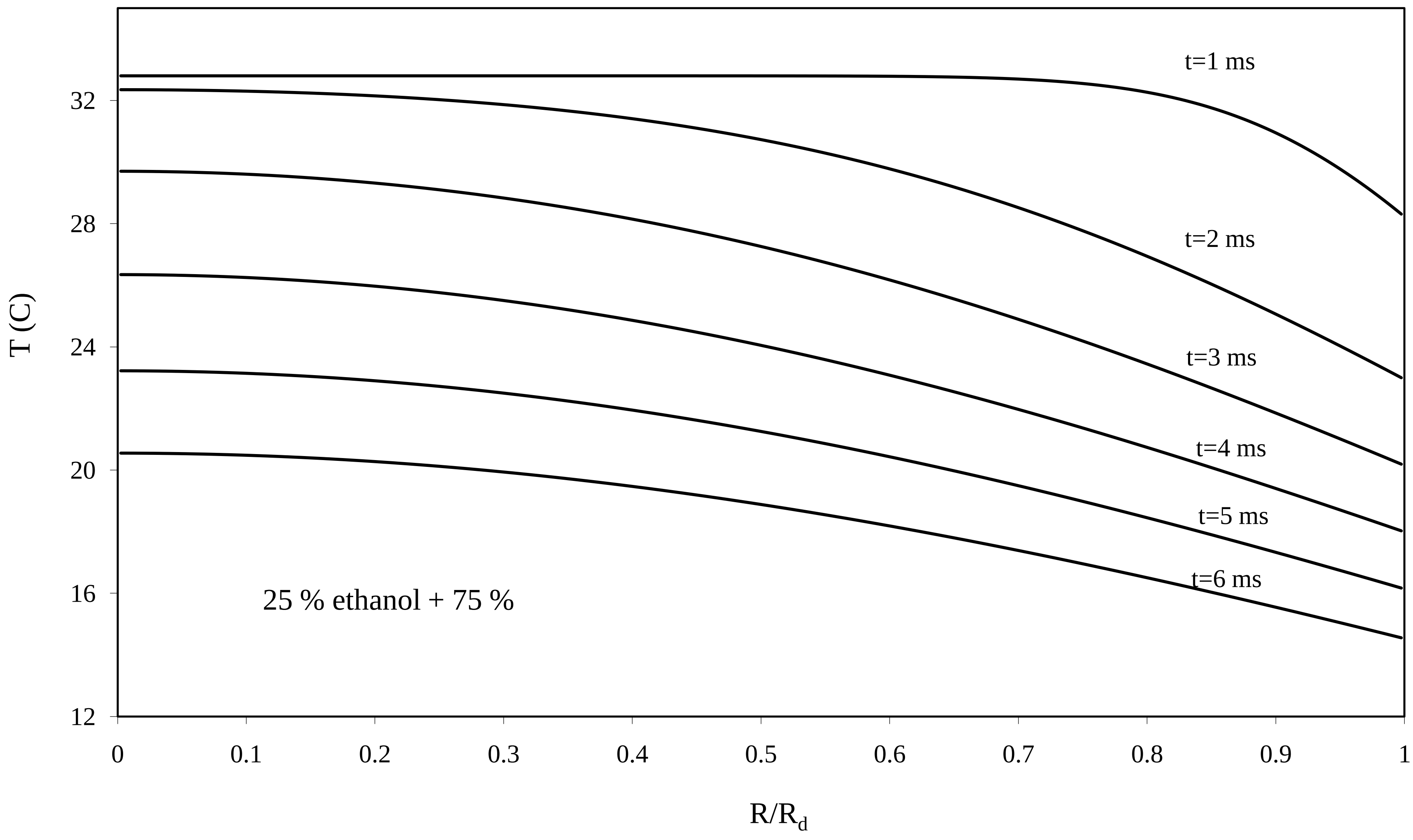


40
35
30
25
20
15
10
T (C)
0
1
2
3
4
5
6
7
Time (ms)
Experiment
Oneway_Sol_Ts
Oneway_Sol_Tav
Vortex model_Ts
Vortex model_Tav
25 % ethanol - 75 % acetone

Results


25 % ethanol + 75 % acetone
t=1 ms
t=2 ms
t=3 ms
t=4 ms
t=5 ms
t=6 ms
$Y_{l,eth}$
R/R_d
0.29
0.28
0.27
0.26
0.25
0.24
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Results


t=1 ms
t=2 ms
t=3 ms
t=4 ms
t=5 ms
t=6 ms
25 % ethanol + 75 %
T (C)
32
28
24
20
16
12
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
R/R$_d$

Conclusions

- A simplified model for bi-component droplet heating and evaporation, based on a new analytical solution of the species diffusion equation, is suggested.

- The predictions of the model have been validated against experimental data referring to measurements of average temperatures and radii of mono-disperse bi-component droplets, and predictions of the vortex model.

A paper is submitted to International Journal of Heat and Mass Transfer.

Thank you for your attention

Your questions are more than welcome

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