A MODEL FOR MONO- AND MULTI-COMPONENT DROPLET HEATING AND EVAPORATION AND ITS IMPLEMENTATION INTO ANSYS FLUENT

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Introduction:

A model for heating and evaporation of mono- and multi-component droplets, based on analytical solutions to the heat transfer and species diffusion equations in the liquid phase, is applied to the analysis of pure acetone, ethanol, and mixtures of acetone/ethanol droplets.

The heat transfer inside the droplet, described by the one-dimensional heat transfer equation, assuming all processes are spherically symmetric;

$$T(r,t) = \frac{1}{r}\sum_{n=1}^{\infty}\left\{\left(I_n - \frac{R_d \sin\lambda_n}{\lambda_n^2}\zeta(0)\right)\frac{\exp(-\kappa\lambda_n^2 t)}{b_n} - \frac{R_d \sin\lambda_n}{b_n\lambda_n^2}\int_0^t \frac{d\zeta(t)}{d\tau}\exp\left(-\kappa\lambda_n^2(t\tau)\right)d\tau\right\}\sin\left[\lambda_n\frac{r}{R_d}\right] + T_{\text{eff}}(t)$$

where r is distance from the droplet centre, R_d is droplet radius, λ_n are positive solutions to the eigenvalue equation where numeration starts from the first positive root, the roots are in ascending order:

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

$$b_n = \frac{1}{2}\left(1 + \frac{h_0}{h_0^2+\lambda_n^2}\right),\ I_n = \int_0^{R_d}\frac{r}{R_d}T(r,0)\sin\left[\lambda_n\frac{r}{R_d}\right]dr,\ h_0 = \frac{hR_d}{k_{\text{eff}}} - 1,\ h = \frac{k_g\,\text{Nu}}{2\,k_{\text{eff}}},$$

$T(r,0)$ is initial temperature distribution inside the droplet, simplifying the heat transfer equation as;

$$T(r,t) = \frac{1}{r}\sum_{n=1}^{\infty}\left\{\left(I_n - \frac{R_d\sin\lambda_n}{\lambda_n^2}\zeta(0)\right)\frac{\exp(-\kappa\lambda_n^2 t)}{b_n}\sin\left(\lambda_n\frac{r}{R_d}\right)\right\} + T_{\text{eff}}(t)$$

Assuming all processes are spherically symmetric. The analytical solution to this equation for the mass fractions Y_i is presented as:

$$Y_i(r,t) = \varepsilon_i + \frac{1}{r}\left[\frac{1}{b_{y0}}\exp\left[D_{\text{eff}}\left[\frac{\lambda_0}{R_d}\right]^2 t\right]\left(I_{i0} + \varepsilon_i\frac{1}{\lambda_0^2}(1+h_{Y0})\sinh\lambda_0\right)\sinh\left(\lambda_0\frac{r}{R_d}\right) + \sum_{n=1}^{\infty}\frac{1}{b_{Yn}}\exp\left[-D_{\text{eff}}\left(\frac{\lambda_n}{R_d}\right)^2 t\right]\left(I_{in} - \varepsilon_i\frac{1}{\lambda_n^2}(1+h_{Y0})\sin\lambda_n\right)\sin\left(\lambda_n\frac{r}{R_d}\right)\right]$$

where λ_0 and λ_n are solutions to the eigenvalue equations:

$$\lambda_0\cosh\lambda_0 + h_{Y0}\sinh\lambda_0 = 0,\ \lambda_n\cos\lambda_n + h_{Yn}\sin\lambda_n = 0,\ (n = 1,2,\ldots)$$

$$D_{\text{eff}} = \left(1.86 + 0.86\tanh\left(2.225\log\left(\frac{\text{Pe}_l}{30}\right)\right)\right)D_l$$

Table 1: Droplet and gas temperatures, droplet diameters and approximations of droplet velocities used in calculations.

Composition	Droplet temperature (K)	Droplet diameter (μm)	Gas temperature (K)	Droplet velocity approximations in m/s (t is in ms)
acetone	308.25	143.4	294.65	12.81 – 0.316t
ethanol	311.15	140.8	295.15	12.30 – 0.344t
25% ethanol	305.65	133.8	294.25	12.75 – 0.370t
50% ethanol	310.65	142.7	293.95	12.71 – 0.488t
75% ethanol	311.75	137.1	294.75	12.28 – 0.306t

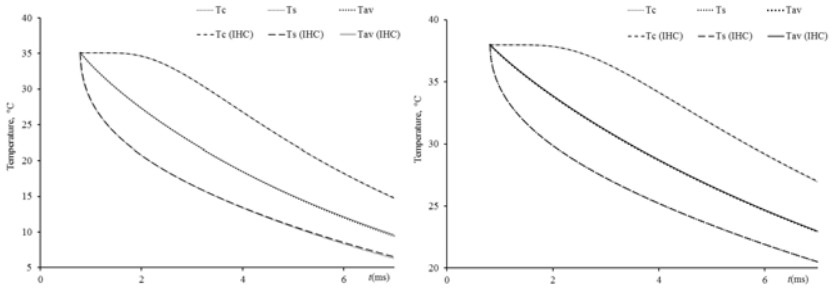

Figure 1a. Time evolution of an acetone droplet **Figure 1b.** Time evolution of ethanol droplet. Surface, average and centre temperatures respectively (T_s, T_{av} and T_c) (see Table 1). ANSYS Fluent results compared with the previously developed In house code.

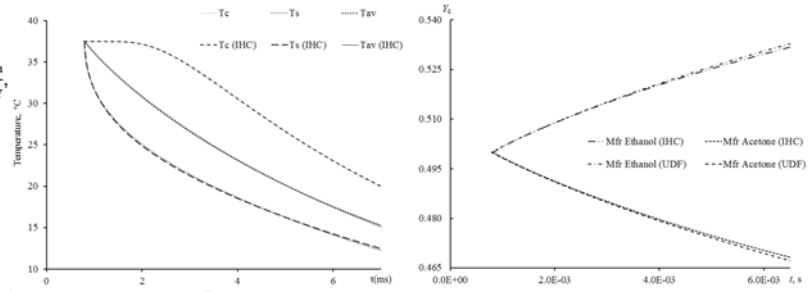

Figure 2a. Time evolution of 50% ethanol 50% acetone droplet surface, average and centre temperatures (T_s, T_{av} and T_c) (see Table 1). ANSYS Fluent results compared with previously developed In house code **Figure 2b**. Time evolution of average component mass fractions for a 50% ethanol 50% acetone droplet.

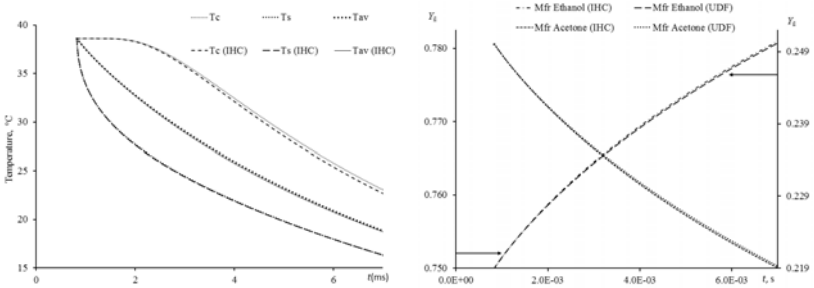

Figure 3a. Evolution of 75% ethanol and 25% acetone droplet surface, average and centre temperatures (T_s, T_{av} and T_c) (see Table 1). ANSYS Fluent results compared with previously developed In house code. **Figure 3b.** Time evolution of average component mass fractions for a 75% ethanol and 25% acetone droplet.

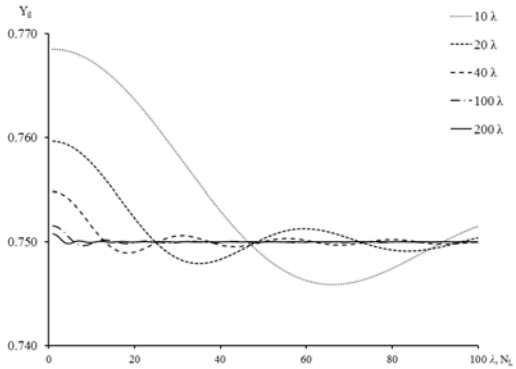

Figure 4. Comparison of the number of terms used for the Eigen value equation lambdas for the first 100 (of 500) layers of an acetone droplet in the first time step.

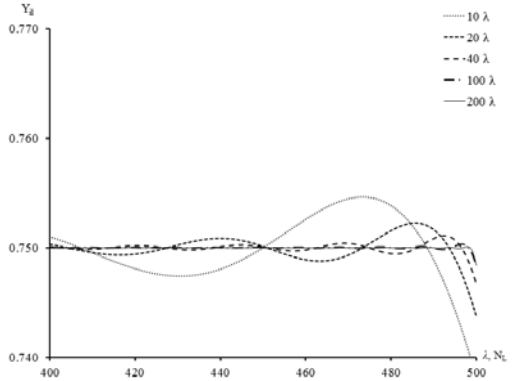

Figure 5. Comparison of the number of terms used for the Eigen value equation lambdas for the last 100 (of 500) layers of an acetone droplet in the first time step.

Conclusions:

The predictions of the customised version of ANSYS Fluent with the new model implemented are compared against the results predicted by the previously developed one-dimensional in-house code.

The agreement between the predictions of these codes is shown to be reasonably good between 0%-2% for mono-component and multi-component droplets.

This gives us confidence in using the new customised version of ANSYS Fluent for the analysis of more complex engineering processes.

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