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Modelling and experimental studies of aerosols and sprays for medical and automotive applications

Multi-component model of droplet heating and evaporation and its implementation into ANSYS Fluent

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Mansour Al Qubeissi, Ahmed Elwardany,

Sergei Sazhin

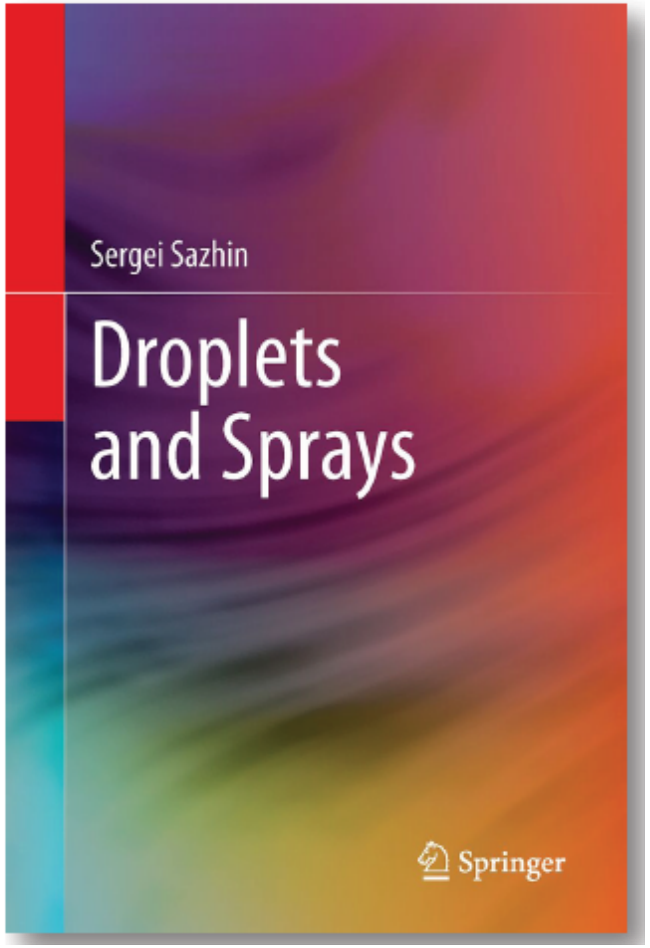
Outline

- Background
- Mathematical formulation
- Validation
- Conclusions

Types of sprays

Fuel Sprays

Medical Sprays



S. S. Sazhin, Modelling of fuel droplet heating and evaporation: Recent results and unsolved problems, Fuel 196 (2017) 69 – 101.

Background

International Communications in Heat and Mass Transfer 76 (2016) 265–270

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HEAT and MASS TRANSFER

A model for droplet heating and its implementation into ANSYS Fluent☆

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Mathematical formulation. Temperature

$$c_{pl} m_d \frac{dT}{dt} = 2\pi \mathrm{Nu} k_g R_d \left(T_g - T_s\right) + L\dot{m}_d + q_{\mathrm{int}}$$

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

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

$$\kappa = k_l / (c_l \rho_l)$$

Mathematical formulation. Temperature

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

$$\left. - \frac{R_d \sin\lambda_n}{b_n\lambda_n^2}\int_0^t \frac{d\zeta(\tau)}{d\tau}\exp\left(-\kappa\lambda_n^2(t-\tau)\right)d\tau\right\}$$

$$\sin\left(\lambda_n \frac{r}{R_d}\right) + T_{\text{eff}}(t),$$

Mathematical formulation. Temperature

$$\lambda \cos \lambda + j \sin \lambda = 0$$

$$b_n = \frac{1}{2}\left(1 + \frac{j}{j^2 + \lambda_n^2}\right), \; I_n = \int_0^{R_d} \frac{r}{R_d} T_0(r) \sin\left(\lambda_n \frac{r}{R_d}\right) dr,$$

$$\kappa = \frac{k_{\text{eff}}}{c_{pl}\rho_l R_d^2}, \; \zeta(t) = \frac{h T_{\text{eff}}(t) R_d}{k_{\text{eff}}}, \; T_{\text{eff}} = T_g + \frac{\dot{m}_d L}{2\pi R_d \text{Nu} k_g}$$

$$j = \frac{h R_d}{k_{\text{eff}}} - 1, \; h = \frac{k_g \text{Nu}}{2R_d}, \; k_{\text{eff}} = \chi k_l$$

Mathematical formulation. Temperature

$$\chi = \left(1.86 + 0.86\ \tanh\left(2.225\quad \lg \frac{\mathrm{Pe}}{30}\right)\right)$$

$$\mathrm{Pe} = 0.79\left|\mathbf{v}_g - \mathbf{v}_d\right| \frac{\mu_g}{\mu_l} \frac{\mathrm{Re}_d^{1/3}}{1 + B_M} \frac{\rho_l R_d c_{pl}}{k_l},\ \ \mathrm{Re}_d = \frac{2R_d \rho_g \left|\mathbf{v}_g - \mathbf{v}_d\right|}{\mu_g}$$

$$B_M = (Y_{vs} - Y_{v\infty})/(1 - Y_{vs})$$

Mathematical formulation. Temperature

$$\mathrm{Nu} = \frac{\ln\left(1 + B_T\right)}{B_T}\mathrm{Nu}^*,$$

$$\mathrm{Nu}^* = 2 + \frac{\left(1 + \mathrm{Re}_d\,\mathrm{Pr}\right)^{1/3}\max\left(1, \mathrm{Re}_\mathrm{d}^{0.077}\right) - 1}{F\left(B_T\right)},$$

$$\mathrm{Sh}^* = 2 + \frac{\left(1 + \mathrm{Re}_d\mathrm{Sc}\right)^{1/3}\max\left(1, \mathrm{Re}_\mathrm{d}^{0.077}\right) - 1}{F\left(B_M\right)},$$

$$F(B_{T,M}) = (1 + B_{T,M})^{0.7}\frac{\ln\left(1 + B_{T,M}\right)}{B_{T,M}}, \quad B_T = (1 + B_M)^{\phi} - 1$$

$$\phi = \frac{c_{pv}\rho_g D}{k_g}\frac{\mathrm{Sh}^*}{\mathrm{Nu}^*}, \quad \mathrm{Pr} = \frac{c_{pg}\mu_g}{k_g}, \quad \mathrm{Sc} = \frac{\mu_g}{\rho_g D}.$$

Mathematical formulation. Species diffusion

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

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

$$\alpha = \frac{|\dot{m}_d|}{4\pi \rho_l R_d^2} \qquad \varepsilon_i = \frac{Y_{\mathrm{vs},i}}{\sum_i Y_{\mathrm{vs,i}}}$$

Mathematical formulation. Species diffusion

$$Y_{\mathrm{l},i} = \varepsilon_i + \frac{1}{R}\left\{\exp\left[D_\mathrm{l}\left(\frac{\lambda_0}{R_\mathrm{d}}\right)^2 t\right][q_{Yi0} - Q_{Y0}\epsilon_i]\sinh\left(\lambda_0\frac{R}{R_\mathrm{d}}\right)\right.$$

$$\left.+\sum_{n=1}^{\infty}\left[\exp\left[-D_\mathrm{l}\left(\frac{\lambda_n}{R_\mathrm{d}}\right)^2 t\right][q_{Yin} - Q_{Yn}\epsilon_i]\sin\left(\lambda_n\frac{R}{R_\mathrm{d}}\right)\right]\right\},$$

$$\tanh\lambda = -\frac{\lambda}{h_{Y0}} \qquad \text{and} \qquad \tan\lambda = -\frac{\lambda}{h_{Y0}}$$

$$h_{Y0} = -\left(1 + \frac{\alpha_m R_\mathrm{d}}{D_\mathrm{l}}\right)$$

Mathematical formulation. Species diffusion

$$Q_{Yn} = \begin{cases} -\frac{1}{||v_{Y0}||^2}\left(\frac{R_\mathrm{d}}{\lambda_0}\right)^2 (1+h_{Y0})\sinh\lambda_0 & \text{when} \quad n=0 \\ \frac{1}{||v_{Yn}||^2}\left(\frac{R_\mathrm{d}}{\lambda_n}\right)^2 (1+h_{Y0})\sin\lambda_n & \text{when} \quad n\geq 1 \end{cases}$$

$$q_{Yin} = \frac{1}{||v_{Yn}||^2}\int_0^{R_\mathrm{d}} R Y_{\mathrm{li}0}(R) v_{Yn}(R)\mathrm{d}R$$

$$v_{Y0}(R) = \sinh\left(\lambda_0 \frac{R}{R_\mathrm{d}}\right), \quad v_{Yn}(R) = \sin\left(\lambda_n \frac{R}{R_\mathrm{d}}\right), \quad n \geq 1$$

Mathematical formulation. Species diffusion

$$||v_{Y0}||^2 = \int_0^{R_\mathrm{d}} v_{Y0}^2(R)\mathrm{d}R = -\frac{R_\mathrm{d}}{2}\left[1 + \frac{h_{Y0}}{h_{Y0}^2 - \lambda_n^2}\right]$$

$$||v_{Yn}||^2 = \int_0^{R_\mathrm{d}} v_{Yn}^2(R)\mathrm{d}R = \frac{R_\mathrm{d}}{2}\left[1 + \frac{h_{Y0}}{h_{Y0}^2 + \lambda_n^2}\right], \quad n \geq 1$$

$$D_\mathrm{eff} = \chi_Y D_\mathrm{l}$$

$$\chi_Y = 1.86 + 0.86 \tanh\left[2.225 \log_{10}\left(\mathrm{Re}_{\mathrm{d(l)}}\mathrm{Sc}_\mathrm{l}/30\right)\right]$$

$$\mathrm{Sc}_\mathrm{l} = \nu_\mathrm{l}/D_\mathrm{l}$$

Validation of the implementation into ANSYS Fluent: Bi-component droplet: acetone+ethanol

Composition	T_{d0} (K)	d_0 (μm)	T_g (K)	v_d (m/s)
25% ethanol	305.65	133.8	294.25	12.75
50% ethanol	310.65	142.7	293.95	12.71
75% ethanol	311.75	137.1	294.75	12.28

A. E. Elwardany, I. G. Gusev, G. Castanet, F. Lemoine, S. S. Sazhin, Mono- and multi-component droplet cooling/heating and evaporation: Comparative analysis of numerical models, Atomization and Sprays 21 (11) (2011) 907–931.

Validation of the implementation into ANSYS Fluent: Bi-component droplet: acetone+ethanol

Composition	Error (T_d)	Error ($Y_{ls,e}$)	Error ($Y_{ls,a}$)
25% ethanol	0.1636%	0.3647%	0.1726%
50% ethanol	0.1423%	0.1730%	0.3110%
75% ethanol	0.1294%	0.2759%	0.7933%

A. E. Elwardany, I. G. Gusev, G. Castanet, F. Lemoine, S. S. Sazhin, Mono- and multi-component droplet cooling/heating and evaporation: Comparative analysis of numerical models, Atomization and Sprays 21 (11) (2011) 907–931.

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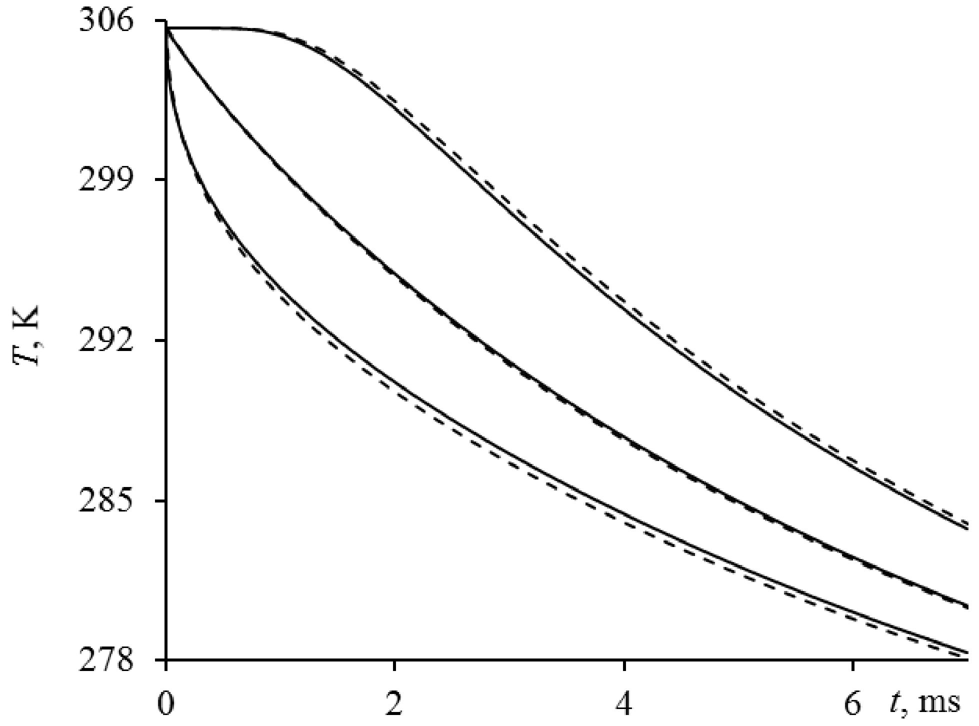
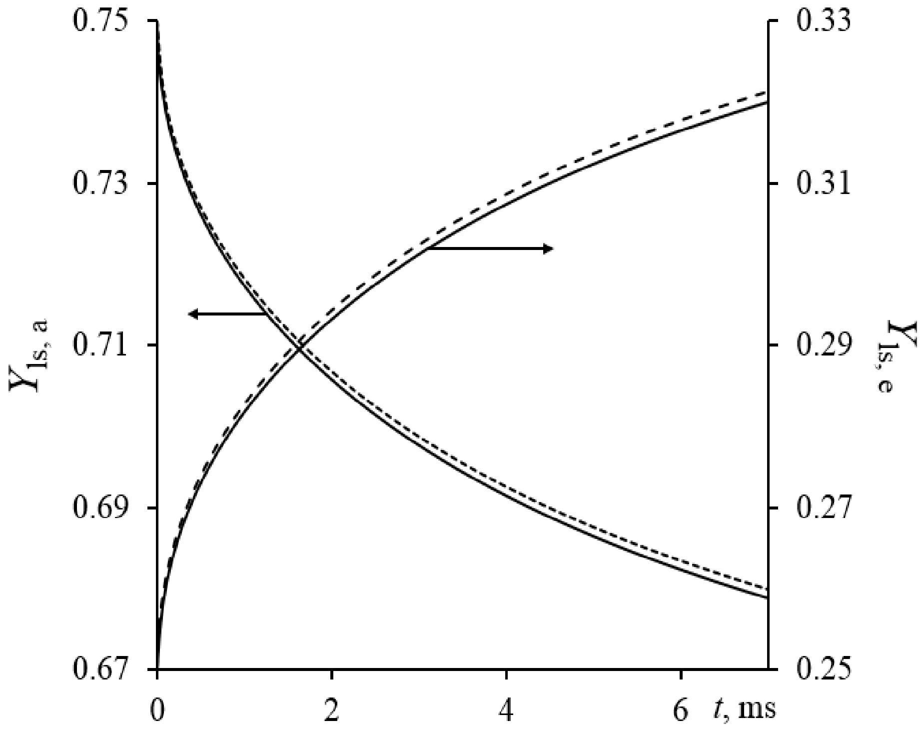
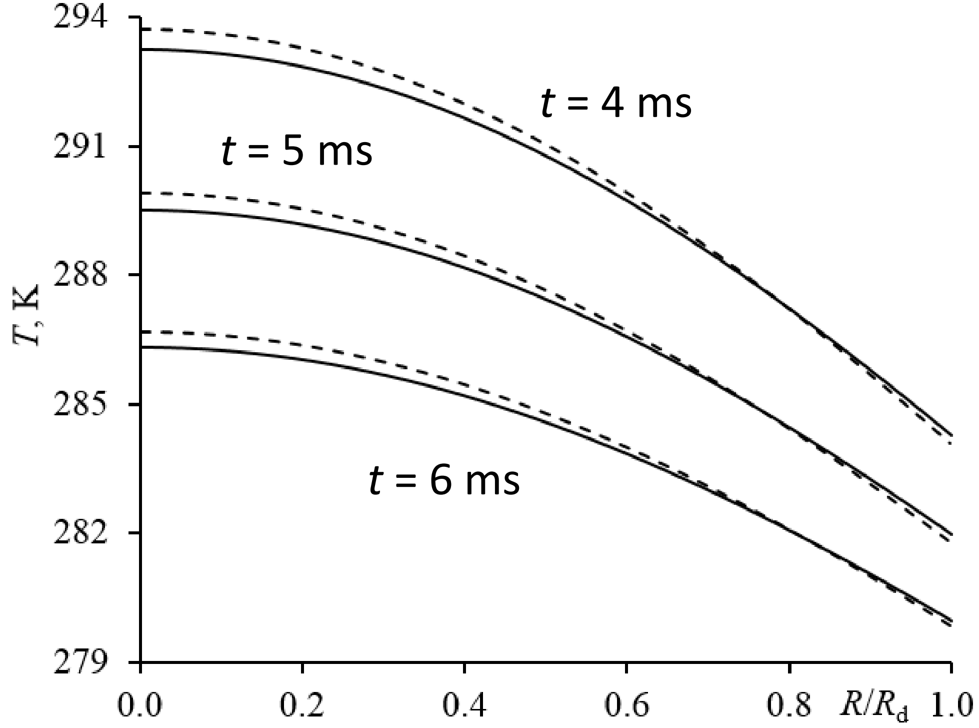
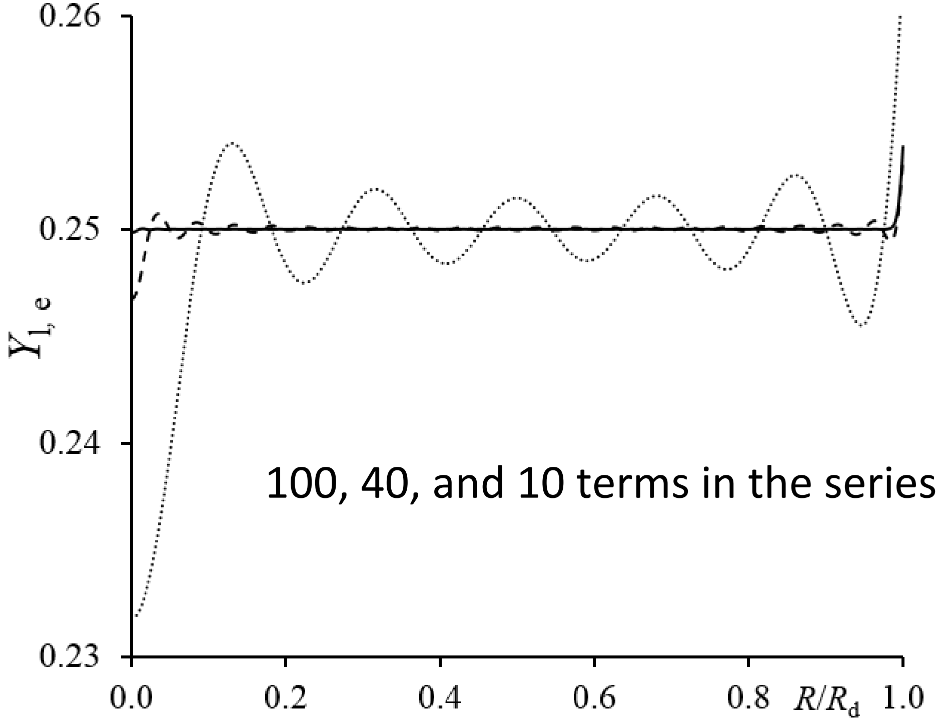




25% ethanol/75% acetone

Validation of the implementation into ANSYS Fluent: Bi-component droplet: acetone+ethanol





25% ethanol/75% acetone

$t = 10^{-5}$ s

Conclusion

- A model for heating and evaporation of multi-component droplets, based on analytical solutions to the heat transfer and species diffusion equations in the liquid phase, has been summarised.
- The model was implemented into ANSYS Fluent via User-Defined Function (UDF).
- The model was applied to the analysis of the mixtures of acetone/ ethanol droplet heat- ing/cooling and evaporation.
- The predictions of the customised version of ANSYS Fluent, with the new model implemented into it, are verified against the results predicted by the previously developed one-dimensional in-house

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