Evaporation of multicomponent fuel droplets in buoyancy driven convection

Abd Essamade Saufi, Eleonora Colombo, Alessio Frassoldati,

Tiziano Faravelli, Alberto Cuoci

Department of Chemistry, Materials and Chemical Engineering, Politecnico di Milano

Abstract

In this work, the evaporation process of multicomponent fuel droplets is analyzed, both from an experimental and numerical point of view. The droplets are hanged on a thin thermocouple against gravity and evaporated in natural convection regime, following the process by means of high speed shadowgraphs. The experimental analyses were performed hierarchically, starting from pure components (n-dodecane and n-hexadecane), then moving to their mixtures. The numerical modeling is performed with the DropletSMOKE++ code, a comprehensive CFD framework for the simulation of 3D evaporating droplets under gravity conditions. The numerical results present a good agreement with the experimental data, especially if compared with the same cased modeled in microgravity conditions. The difference evaporation rate is analyzed as well as the different surface temperature, highlighting the important role of internal and external convection on the evaporation process.

Introduction

The high energy density of liquid fuels is exploited nowadays in many engineering applications such as internal combustion engines, industrial burners and sprays. The study of the complex interacting phenomena occurring among this large amount of droplets is essential, but still too complex to be handled. In order to simplify the problem, isolated droplets are usually studied. The microgravity condition allows a relatively simple modeling, since 1D geometry is established and because many effects such as natural convection and droplet deformation can be easily neglected. However, in most of the engineering applications these phenomena are important and they often control the physics of the problem [1]. The drawback is that in this case the mathematical modeling is more complicated, since the droplet has a 3D geometry and it is deformable. Moreover, the liquid and gas phase velocity fields have to be calculated in order to account for external convection and internal liquid circulations, which are known to be fundamental phenomena for a correct modeling of evaporating droplets [2]. In this work the experiments from Han et al. [3] are analyzed, involving multicomponent droplets evaporating in natural convection regime at different temperatures. The numerical simulations are performed with the DropletSMOKE++ code, a multiphase CFD solver developed at Politecnico di Milano, based the VOF methodology to dynamically track the liquid interface [4]. The experiments are also modeled using the 1D code by Cuoci et al. [5], in order to highlight the effect of external and internal flow field on the evaporation process.

Mathematical modeling

The VOF (Volume Of Fluid) methodology has been adopted [6], in which a step function α tracks the liquid volume fraction. The solver is based on the OpenFOAM 4.x framework. The transport equation for α is here reported:

corresponding author: Abd Essamade Saufi abdessamade.saufi@polimi.it

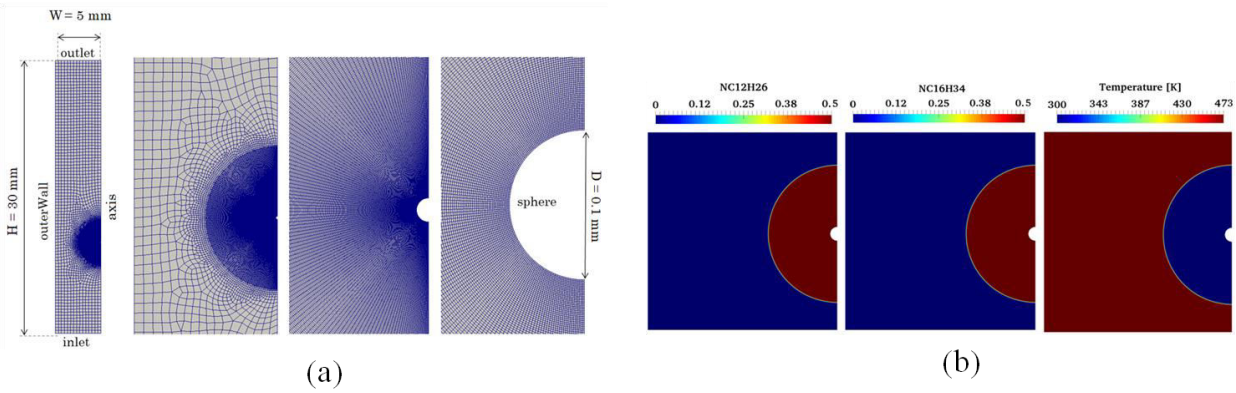

Figure 1: Computational mesh at four different levels of detail (a). N-dodecane, n-hexadecane mass fractions and temperature initial conditions (b).

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \vec{v}) = -\frac{\dot{m}}{\rho_L} - \frac{1}{\rho_L}\frac{D\rho_L}{Dt} \tag{1}$$

The source terms represent evaporation and liquid density variations. The transport properties are weighted by the α function. The momentum equation describes the whole flow field:

$$\frac{\partial \rho \vec{v}}{\partial t} + \nabla \cdot (\rho \vec{v}\vec{v}) = \nabla \cdot \mu\left(\nabla \vec{v} + \nabla \vec{v}^{\mathrm{T}}\right) - \nabla p + \rho \vec{g} \tag{2}$$

while the energy equation provides the temperature field, including the interface cooling:

$$\rho C_p \left(\frac{\partial T}{\partial t} + \nabla \cdot (\vec{v}T)\right) = \nabla \cdot (k \nabla T) - \sum_{i}^{Ns} \dot{m}_i \Delta h_{ev,i} \tag{3}$$

Concerning the species transport, the equation is written only for the saturated mass fraction of each species [7]. A major advantage of the DropletSMOKE++ code is that the evaporating flux is not obtained by semi-empirical laws [8], but it directly depends on the mass flux $\vec{J}_{d,i}$ at the liquid-gas interface:

$$\dot{m}_i = -\frac{\sum_i^{Ns} \vec{J}_{d,i}}{1 - \sum_i^{Ns} \omega_i} \nabla \alpha \tag{4}$$

Where the term $1 - \sum_i^{Ns} \omega_i$ accounts for the Stefan flow induced by evaporation. The α gradient describes the interface surface per unit volume [9] and forces evaporation to happen only at the interface. The transport properties for liquid and gas phases are provided by the OpenSMOKE++ library [10].

Numerical methodology and experimental cases

The domain geometry is 2D, axysimmetric, representing a slice of a cylinder having a radius W = 5 mm and height H = 30 mm (Figure 1 a). The region including the liquid droplet and the gas in its proximity is meshed with a concentric pattern, getting finer while approaching the inner fiber. The mesh is composed by 70,000 cells, fine enough to provide a complete mesh independence. The experimental cases are reported in Table 1. The droplets are hanged on a thin thermocouple and evaporated in natural convection. The fuel mixture is based on n-dodecane and n-hexadecane in equal volumetric fractions (Figure 1 b). The droplet is evaporated at three different ambient temperatures (473 K, 573 K and 673 K).

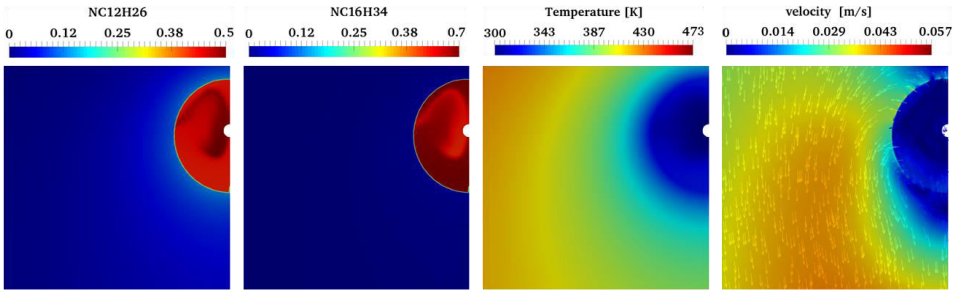

Figure 2: Screenshots of mass fractions of n-dodecane (a), n-hexadecane (b), temperature (c) and vector velocity field (d). Time t = 2 s.

Case	Species	D_0 [mm]	T_L [K]	T_G [K]
1	n-C_{12}/n-C_{16}	0.9	300	473
2	n-C_{12}/n-C_{16}	0.9	300	573
3	n-C_{12}/n-C_{16}	0.9	300	673

Table 1: Experimental cases in natural convection examined in this work.

For each one of the three cases presented in Table 1, an equivalent simulation (e.g. with the same initial conditions) has been performed with the microgravity solver of Cuoci et al. [5] in order to highlight the impact of gravity on the numerical simulation. Figure 2 reports the mass fraction fields of the two fuel species, the temperature and the velocity field at time t = 2 s, for Case 1 (Table 1). The evaporation causes a downward velocity field (because of the higher density of vapor with respect to air) which enhances the heat and mass transfer between the liquid and the gas phase. The consequent internal circulation effectively redistribute the species mass fractions (Figure 2 a, b) and the temperature field (Figure 2 c). The normalized diameter behavior (Figures 3 a, b, c) is well predicted code for the three cases. The 1D model systematically underpredicts the evaporation rate by a factor ~ 2, because of the lower heat and mass transfer coefficients due to the absence of external convection. Whereas this difference is evident concerning the squared diameter decay, the surface temperature seems to be less affected. The predicted steady-state temperature (wet-bulb) is the same for the two models, indicating an independence on the external convection [4]. However, the droplet surface is heated faster in natural convection than in microgravity, due to the enhanced heat transfer. It is worth noticing that for Cases 2, 3 in Figures 3 (e, f) the surface temperature shows two steady-states values, typical of the differential evaporation phenomenon: the light species (n-dodecane) evaporates faster than the heavy one (n-hexadecane) providing a two steps evaporation. This effect is further enhanced with the increase of the external temperature.

Conclusions

The DropletSMOKE++ code has been adopted to model the evaporation of 3D multicomponent droplets under natural convection regime. The VOF method has been used to track the liquid interface and it is coupled with the solution of a velocity, temperature and mass fraction field. The external gas flow causes internal recirculation in the liquid phase, because of the external applied shear stress. The comparison with the 1D model shows a large difference between the two models, better supporting the need of a multiphase CFD code to model these systems.

Future developments concern the activation of gas-phase reactions, as well as the analysis on the effect of the supporting thermocouple on the evaporation process.

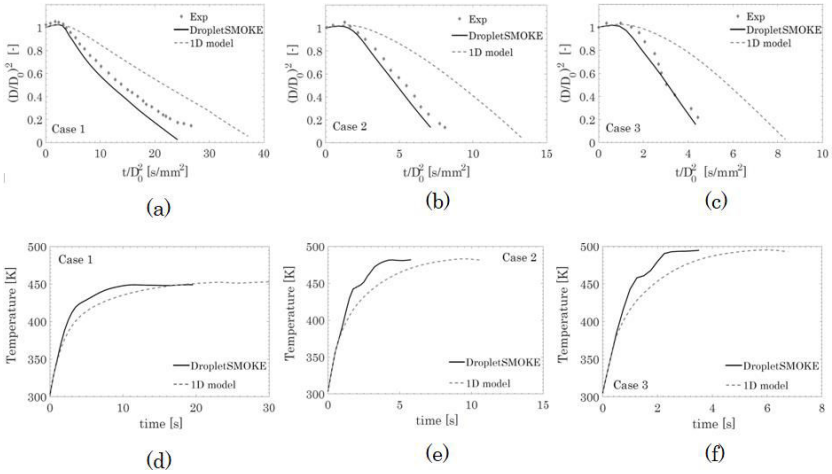

Figure 3: Comparison between DropletSMOKE++ results, experiments and the 1D model for cases in Table 1. Normalized diameter (Figures a, b, c) and surface temperature (Figures d, e, f).

Acknowledgments

The authors acknowledge the support by the European Union's Horizon 2020 research and innovation program (Residue2Heat, G.A. No. 654650).

References

[1] Soh et al. "An algorithm to calculate interfacial area for multiphase mass transfer through the VOF method" *Int. Journal of Heat and Mass transfer* 100, 573-581 (2016)

[2] Jaeheon S. et al. "A computational study of droplet evaporation with fuel vapor jet ejection induced by localized heat sources" *Physics of Fluids* 27, (2015)

[3] Han K. et al. "Experimental and theoretical study of the effect of suspended thermocouple on the single droplet evaporation" *Appl.Thermal Eng.* 101, 568-575 (2015)

[4] Saufi A.E. et al. "DropletSMOKE++: a multiphase computational framework for the evaporation of multidimensional fuel droplets" *Int. J. Heat and Mass Transfer*, (2018)

[5] Cuoci A. et. al. "Autoignition and burning rates of fuel droplets under microgravity" *Comb. and Flame* 143, 211-226 (2005)

[6] Hirt C.W., Nichols B.D., "VOF Method for the Dynamics of Free Boundaries", *Journal Of Computational Physics* 39, 201-225 (1981)

[7] Banerjee R. "An algorithm to determine the mass transfer rate from a pure liquid surface using the VOF multiphase model" *Int. Journal Engine Research* (2004)

[8] Nabil M., Rattner S. A., " A framework for two-phase flow simulations with thermally driven phase change" *SoftwareX* 5, 216-226 (2016)

[9] Soh G.Y. et al. "An algorithm to calculate interfacial area for multiphase mass transfer through the VOF method" *Int. Journal of Heat and Mass transfer* 100, 573-581 (2016)

[10] Cuoci et al. "OpenSMOKE++: An object-oriented framework for the numerical modeling of reactive systems with detailed kinetic mechanisms "*Computer Physics Communications* 192, 237-264 (2015)