# A CFD FRAMEWORK FOR EVAPORATING FUEL DROPLETS IN A GRAVITY FIELD

**A.E. Saufi, A. Cuoci, A. Frassoldati, T. Faravelli**
abdessamade.saufi@polimi.it
Dip. Chimica, Materiali e Ingegneria Chimica, Politecnico di Milano, 20133 Milano, Italy

**Abstract**
A comprehensive CFD model for the simulation of evaporating droplets under gravity conditions is here presented. The model is based on the Volume Of Fluid (VOF) methodology [1], which allows an accurate tracking of the gas-liquid interface with excellent mass conservation properties. The whole flow and temperature field are given by a single momentum and energy equation valid for both phases. Three numerical simulations are presented: an assessment of mass conservation of the CFD code and a comparison between the absence and the presence of a gravity field in the evaporation of a n-heptane droplet. A final section on the presence of internal recirculation in the liquid phase is also presented.

## Introduction

The high energy density of liquid fuels is exploited nowadays in many engineering applications such as internal combustion engines, industrial burners and sprays. In these systems the fuel is used after a proper atomization, in order to minimize pollution problems and increase the efficiency. 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, both from an experimental and numerical point of view. Numerous analyses can be found on isolated droplets evaporation and combustion [3], and they can be divided in two main areas. The first in which microgravity conditions are imposed. The FLEX campaign [3] showed many phenomena regarding isolated droplets in microgravity conditions and the mathematical modeling of these systems it is still a wide and interesting area of research. The microgravity condition allows a relatively simple modeling, since 1D geometry is established and because many effects such as surface tension, 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; the presence of forced or natural convection heavily affects the evaporation rate, as well as the droplet deformation which locally modifies the droplet surface [4]. This is why most of the experiments are done in gravity conditions, which also allow much cheaper experimental devices. The drawback is that in this case the mathematical modeling is more complicated. The droplet has now a 3D geometry, its shape and curvature depend on surface tension. Moreover, the liquid and gas phase velocity field has to be calculated in order to

account for external convection and internal liquid recirculations, which are known to be key phenomena for a correct modeling of droplets [5].
In this work a multiphase CFD model has been developed, exploiting the VOF methodology to dynamically track the liquid interface. This method is a one-fluid approach, widely known for its simplicity, robustness and mass conservation properties. The liquid volume fraction is tracked by a function α, while the interface is advected geometrically [6]. A single equation of motion is written for the whole flow field, modeling therefore a single fluid with step physical properties. This methodology has been successfully implemented to model bubbles growth, liquid films [2] and it is widely used in naval engineering problems.
The main drawback in VOF approach is the modeling of surface tension driven flows. Small droplets (~1-2 mm diameter) have a very large interface curvature, whose value is needed to compute the surface tension force. The numerical evaluation of curvature from α step-function is a numerical challenge and errors in this calculation form unphysical velocities around the interface called parasitic currents, which can easily propagate [9]. Many ways have been proposed to reduce this problem [8], but none of them is able to completely eliminate the parasitic currents, in particular for such small droplets. In order to overcome this problem, a small spherical fiber is place inside the droplet and a centripetal force directed towards its center has been imposed, in order to keep it strongly held to the fiber even when gravity is present. In this system surface tension is not needed anymore and it can be neglected, eliminating parasitic currents directly from their source.

**Mathematical modeling**
The governing equations for the multiphase CFD model are here presented. The VOF methodology has been used, where 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:

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

The liquid volume fraction has a negative source term because of evaporation. The transport properties (thermal conductivity, viscosity and diffusion coefficients) are weighted by the α function. The momentum equation describes the whole flow field:

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

while the energy equation provides the temperature field:

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

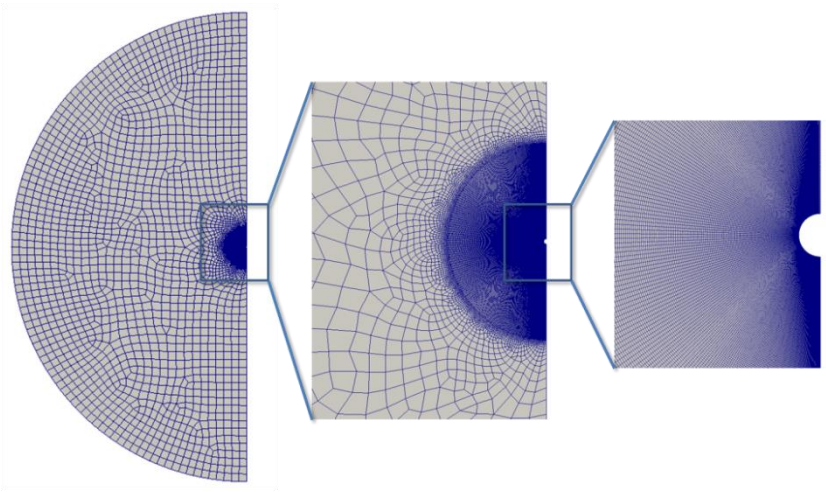

Figure 1: Computational mesh in three different levels of detail. Global geometry (left figure) and fiber (right figure).

Concerning the species transport, the equation is written only for the saturated mass fraction following the approach proposed by Banerjee [10]. The equilibrium vapor mass fraction at the interface is computed through ideal thermodynamics and from the interface is diffused into the gas phase. It is extremely important to correctly model the species diffusion since the evaporating flux is not obtained by semi-empirical laws [2], but it directly depends on the mass fraction gradient at the liquid-gas interface:

$$\dot{m} = -\frac{\rho \mathfrak{D}_i \nabla \omega_i}{1 - \omega_i} \nabla \alpha \tag{4}$$

Where the term $1 - \omega_i$ accounts for the Stefan flow induced by evaporation. The α gradient describes the interface surface per unit volume [4] and forces evaporation to happen only at the interface (where the gradient is different from zero). Equation (4) also accounts for the cooling of the surface when evaporation occurs.
All the transport properties for liquid and gas phases are given by the OpenSMOKE++ library [11], developed at Politecnico di Milano.

**Setup of the numerical simulation**
The computational mesh describes an axisymmetric domain (Figure 1), where only a 5° angle of a global spherical geometry is accounted for. The domain diameter is 50 mm, while the liquid droplet (placed at the center of the domain) diameter is 1

mm. Inside the droplet a spherical fiber (d = 0.1 mm) is placed. The mesh is made by 110,000 cells, chosen by a sensitivity analysis on the cells size. The time step is controlled by the Courant number (< 1) .
The initial droplet diameter is 1 mm for all the simulations and the fuel is n-heptane.

**Monocomponent droplet evaporation**

In this work three simulations are presented: the first one is done in microgravity conditions, only to verify the correct mass conservation of the code. A fixed mass flux $\dot{m}$ is imposed and the diameter behavior in time given by the CFD code is compared with the simple analytical solution $D(t) = \sqrt[3]{D_0^3 - \frac{6\dot{m}}{\rho\pi}t}$

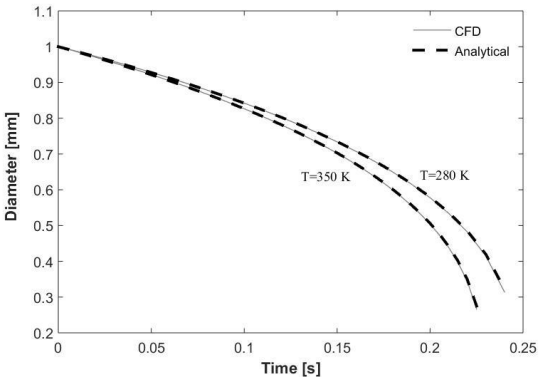


Figure 2: Diameter vs. time plot for two different temperatures. CFD results vs. analytical solution.

The results are shown in Figure 2 showing a good agreement with the given analytical solution. This is a key simulation in order to assess if the source term in equation (1) is correctly implemented. This has been done for two temperatures ( T = 350 K and T = 280 K) to verify the effect of the consequent difference in the liquid density. The other two simulations concern the diffusion controlled evaporation of a liquid droplet of n-heptane in microgravity and in gravity conditions. In Figure 3 we can see the liquid volume fraction field α, the fuel mass fraction and the velocity field for the two simulations. Differently from the 1D codes, the CFD simulation can provide an immediate visualization of the vapor cloud which is formed around the droplet during the evaporation. When gravity is present, an important velocity field is formed because of the high density difference between the air and the released heptane vapor which heavily modifies the cloud shape around the droplet.

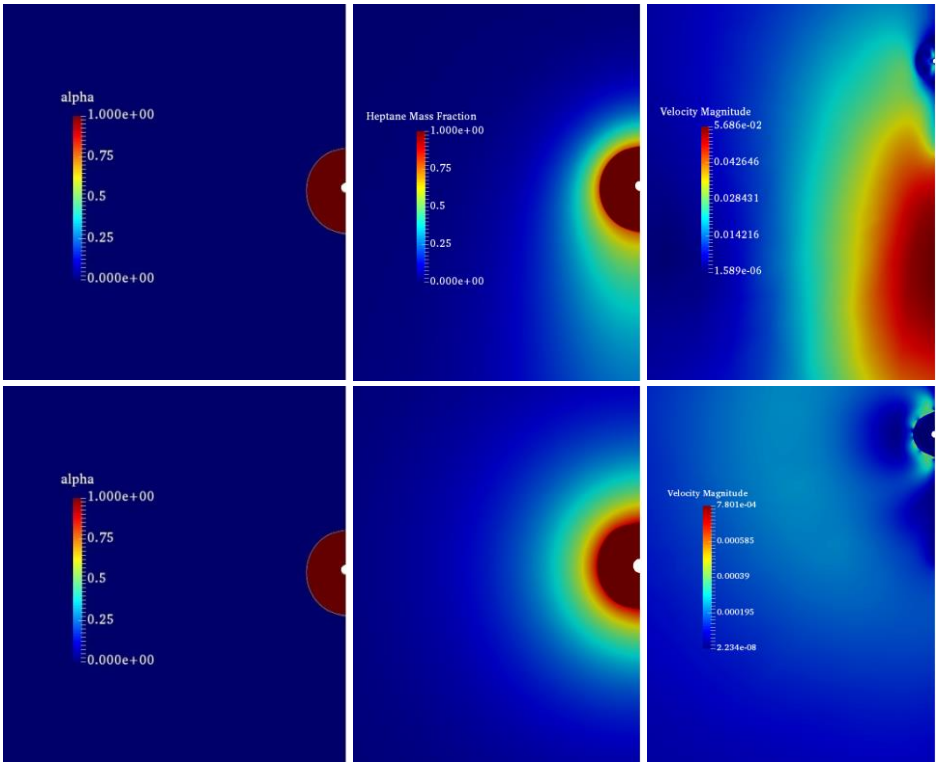


Figure 3: Liquid volume fraction α (left), fuel mass fraction (middle) and velocity field (right). Simulations in gravity (top) and microgravity (bottom) conditions.

**Internal liquid recirculations**

1D codes for the modeling of droplets evaporation usually suffer from an under estimation of the heat transfer from the gas to the liquid phase [3]. This is because 1D model cannot predict the internal recirculations, caused by temperature or concentration gradients and by the shear stress on the liquid surface given by the external gas motion. In the presented model the liquid velocity field is naturally included in the solution of Equation (2), as can be seen in Figure 4. The net effect of this velocity field is the higher internal mixing which enhances heat and mass transfer.

**Conclusions and future developments**

A three-dimensional CFD model for the evaporation of fuel droplets has been developed. The VOF method has been used to track the liquid interface and it is coupled with the solution of a velocity, temperature and concentration field. The presence of gravity induces natural convection around the droplet modifying the vapor cloud shape. The external gas flow also causes internal recirculation in the liquid phase, because of the external applied shear stress.

Future developments concern the validation of the evaporative model with experimental data and the activation of gas-phase reactions.

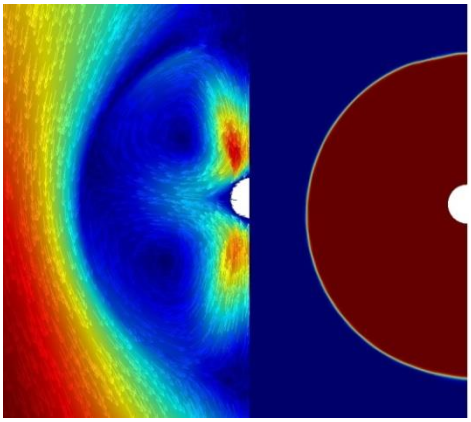

Figure 4: Liquid volume fraction α (right) and velocity field [0-2 cm/s] inside and outside the droplet during the evaporation (left).

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