

# Modelling of a Diesel Oil Spray at Different Swirl Numbers and Comburent Temperature in Mild Combustion Conditions

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Since the combustion of liquid fuel is a very complex phenomenology, usually realized with interactions between a two phase flow and with high number of chemical reactions, we analysed the phenomena related to the problem to well understand the condition for a good mixing process in a combustion chamber, using an applied fluid-dynamic analysis approach type.

Particularly, the local concentration profile of droplet jets, both in spatial and in time coordinate, at some significant station in proximity of the inlet jet's source, besides the stability conditions for a swirling droplet jet case, has been studied.

Starting from the experience acquired in the field related to liquid fuel and well exposed in scientific literature (D'Alessio, Sommerfeld, Cuenot, Peters), this paper analyzes some aspects concerning the behaviour of a fuel spray in a combustion chamber at different injection conditions, using a CFD commercial code for the simulations.

## 1. Introduction

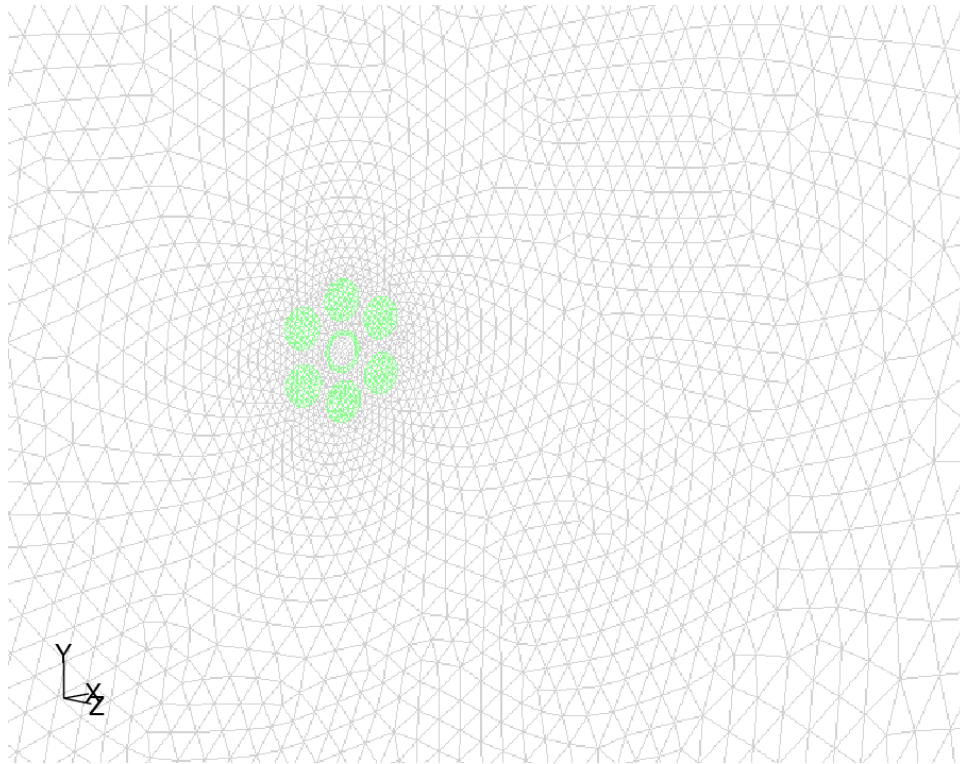
Mild combustion is a particular combustion technique characterized by both an elevated temperature of reactants in the hypothesis of the presence of an adiabatic flame temperature not higher than 1600 K.

The increase of reactants temperatures and oxygen dilution in the comburent are usually thought to be beneficial in the combustion conversion to CO<sub>2</sub> and H<sub>2</sub>O.

On the other hand the decrease of adiabatic flame temperature allows reducing soot and NO production. In this work the attention is focused on the possibility to realize a combustion process with both high efficiency and low emissions. There is some experience in the fundamental field related to liquid fuel, which has lead to some well-quoted results in scientific literature, but anyway these experiences are less than theoretical models for gas fuel combustion case.

So we investigated about an approach to a model for mild combustion of liquid fuel, studying the influence of reactants temperature on fuel vaporization and diffusion. More particularly the behaviour of a fuel droplet spray interacting with a comburent flow (air) is

analysed by using a CFD simulation and the determination of fuel concentration map in the comburent flow, varying inlet gas temperature from 300 to 1200 K. As the combustion of liquid fuel is a very complex phenomenology (interactions between a two phase flow and a high number of chemical reactions), very simple burner geometry has been used. Here a swirling fuel spray blows out in a chamber with six channels symmetrically disposed around the nozzle, which provides to the liquid fuel atomisation, in a quiescent environment.



**Fig.1: Fuel and air injection holes**

## **2. Spray Combustion**

The combustion of liquids is typically accomplished by injecting a liquid through an orifice into a gas-phase combustion environment. The emerging liquid stream breaks up into a dense cloud of droplets that penetrate into the combustion zone. Heat transfer to the droplet increases vapour pressure until subsequent gas-phase ignition commences.

Implicit in the study of single droplet combustion is the assumption that combustion of a dense cloud of many droplets emerging from a fuel spray can be viewed as an ensemble of single droplet combustion. This implicit assumption is analogous to the assumption that turbulent flames can be modelled as an ensemble of laminar flames. Both assumptions have lead to an improved understanding of the combustion process. Thus, a detailed understanding of the processes in single droplet combustion is a requirement for the greater understanding of combustion of an ensemble of droplets, i.e., spray combustion.

Great model simplification results when one assumes spherical symmetry, since then the mathematical model becomes one-dimensional. The simulation is performed by solving the conservation equations in the gas phase, the droplet, and at the interface (see, e.g., Cho et al. 1992, Stapf et al. 1991, 1994). This simple system can be realized experimentally when single droplets are injected into a chamber of hot combustion products. In order to avoid

gravitational effects, which perturb the spherical symmetry, the combustion gases are convected downward at the velocity of the droplet, or even better, the combustion chamber is situated in a fall tower where gravity is zero for the short duration while the experiment falls (see, e. g., Yang and Avedisian 1988).

Most liquid fuels are distilled from petroleum and consist of hundreds of compounds with a range of boiling points. As the liquid drop begins to heat up, the most volatile liquids will evaporate first, followed by liquids of intermediate volatility (and thus higher boiling temperature), and then by the vaporization of remaining low volatility (viscous oils). Fortunately, autoignition occurs early in this sequence of events, so the evaporation of the low volatility oils is augmented by the flame that now encircles the remains of the drop.

As noted above, a first step towards modelling of spray combustion is to assume that the burning spray is merely an ensemble of single, non-interacting, burning droplets. The droplets emerge from the jet as a dense cloud of drops with a wide range of diameters. However, it is not known how these different size drops interact with each other and with the turbulent gaseous flow field (see, e.g., Williams 1990). These questions have been addressed by dividing the overall process into the formation of the spray, the motion of the droplets, and evaporation, followed by combustion.

The spray is formed, as a fuel jet (coming, e. g., from a nozzle) is shattered by shear forces during injection. This process is similar to the formation of turbulent structures in shear layers (Clift et al. 1978). The liquid fragments, which are not yet spheres, are launched into the (usually turbulent and recirculating) flow fields of oxidizer and combustion products. The distribution of droplet diameters in a spray is not uniform. It has been profitable to characterize the distribution of diameters by various size distribution functions with associated moments that evolve in time. The distribution function and the subsequent evolution is largely determined by the nature of the injection and the flow in the combustor (i.e., the boundary conditions).

Evaporation of the droplets and diffusion of the fuel into the gas phase leads to the formation of a combustible mixture, which ignites at sufficiently high temperatures.

Chang et al. [2] investigated a hollow-cone spray numerically, where the emphasis was on the validation of the stochastic approach describing turbulent dispersion. Because of the poor agreement of measured and calculated probability density functions (PDFs) of droplet velocity components, the unsuitability of this approach applied to hollow-cone sprays was concluded.

Usually, the increase of the Sauter mean diameter (SMD) along the spray distance was also found by many researchers, and most explanations involved droplet collision followed by coalescence and vaporisation with preferential vaporization of small droplets.

A comprehensive study about the relevance of each process could not be found until now. Among other parameters, the influence of viscosity and surface tension effects may be of importance, as reported by Dorfner et al [3]. These effects are excluded in this study.

The present article aims at a detailed study of different physical effects present in common sprays obtained with a hollow-cone spray nozzle. Special emphasis is laid on the contribution of droplet collision/coalescence and vaporization on the local droplet size distributions, droplet mass fluxes, and the velocity fields of both phases downstream of the nozzle. The experimental results are compared with numerical calculations and used for validating the individual models applied in this study.

The fluid flow was obtained by solving the time-averaged Navier-Stokes equations in connection with the well known  $\kappa$ - $\epsilon$  turbulence model of Launder and Spalding.

The static enthalpy equation and mass transfer equations for evaporated water and air were solved to take into account phase changes due to droplet evaporation.

The fluid density depends on the gas mixture and temperature and is calculated using the ideal gas law. The other fluid properties, such as molecular viscosity  $\mu$ , the thermal conductivity coefficient  $\lambda$ , the diffusion coefficient  $D$ , and the heat capacity  $C_p$ , are also calculated as function of temperature and mixture composition. Additional source terms are introduced to account for the influence of the droplets on the fluid flow.

The resulting set of equations was solved by using a finite volume discretization scheme based on the SIMPLE algorithm of Launder and Spalding, where a staggered grid arrangement was applied.

The dispersed (droplet) phase is treated by the Lagrangian approach, where a large number of droplet parcels, representing a number of real droplets with the same properties, are traced through the flow field. The representation of droplets by parcels is used in order to allow the consideration of a droplet size distribution and simulate the measured liquid mass flow rate at the injection locations by a reasonable number of computational droplets. The trajectory of each droplet parcel is calculate through a step by step integration of the differential equation of motion for a single droplet.

### **3. Dispersion modelling**

The energy transfer which takes place in a droplet dispersion process, in a quiescent environment, or in a combustion chamber where liquid fuel is injected, is completed by a further going away from each other of particles generated.

The transport of these parameters plays an important role in diffusion process and so in the following combustion one; this process requires mixing ratio as uniform as possible, in order to fully take place.

In this contest the present work is set which provide a series of numerical tests in mild combustion conditions. Three families of tests have been carried out for comb rent temperature at 300, 800, and 1200 K.

The nozzle model is made of a central body that injects the fuel and gives a swirling condition to the jet due to high pressure. Droplets are generated in the typical shape of rotating ring; they have all been considered 1  $\mu$  diameter; this simplification was adopted in order to have a typological and qualitative analysis of the phenomenon.

### **4. The CFD code**

A commercial code (Fluent) was adopted to simulate the process of droplet dispersion into the comburent stream, with the aid of some special function finalised to obtain a corrected outlet pressure. In addition to solving transport equations for the continuous phase, the code adopted allows to simulate a discrete second phase in a Lagrangian frame of reference. This second phase consists of spherical particles (which may be taken to represent droplets or bubbles) dispersed in the continuous phase. The CFD code computes the trajectories of these discrete phase entities, as well as heat and mass transfer to/from them. The coupling between the phases and its impact on both the discrete phase trajectories and the continuous phase flow can be included.

The code adopted provides the following discrete phase modelling options:

- Calculation of the discrete phase trajectory using a Lagrangian formulation that includes the discrete phase inertia, hydrodynamic drag, and the force of gravity, for both steady and unsteady flows

- Prediction of the effects of turbulence on the dispersion of particles due to turbulent eddies present in the continuous phase
- Optional coupling of the continuous phase flow field prediction to the discrete phase calculations
- Heating/cooling of the discrete phase, vaporization and boiling of liquid droplets: we don't consider these effects in this case
- At the last the combusting particles process, including volatile evolution and char combustion to simulate coal combustion, that will be the next step of our work

These modelling capabilities allow CFD code to simulate a wide range of discrete phase problems including particle separation and classification, spray drying, aerosol dispersion, bubble stirring of liquids, liquid fuel combustion, and coal combustion. The physical equations used for these discrete phase calculations are described in the following sections.

## 5. Particle transport in turbulent flows

The dispersion of particles due to turbulence in the fluid phase can be predicted using the stochastic tracking model or the particle cloud model. The stochastic tracking model (random walk) includes the effect of instantaneous turbulent velocity fluctuations on the particle trajectories through the use of stochastic methods.

$$\frac{dU_{p,i}}{dt} = \frac{U_i - U_{p,i}}{\tau_p} + g_i \quad [1]$$

$$\text{where} \quad \frac{dx_{p,i}}{dt} = U_{p,i} \quad [2]$$

There are different ways to break up a liquid film into a number of small droplets.

The simulation carried out in this work analyses the case of interaction between the liquid fuel injected and broken up in the nozzle, with a hot air stream, which is responsible of a further break up close to the nozzle itself.

Tests have been performed considering a high tangential component of velocity.

Two types of situation have been modelled: a cold interaction with fuel injected in a calm environment and an hot interaction with fuel broken up into a number of small droplets also by action of hot air jets.

The break up is strongly influenced by disturb to the liquid flow determined by turbulence and by properties of the gaseous medium in which the jet is injected.

In liquid jet with axial flow a simple vibration of the jet is able to determine the break-up.

In literature are well reported a big amount of data about mild combustion of gaseous fuel, less about liquid ones. This work analyses a spray of fuel droplets testing first the validity of different turbulence models (standard, RNG, realizable k-ε), then the interaction with high temperature comburent has been pointed out.

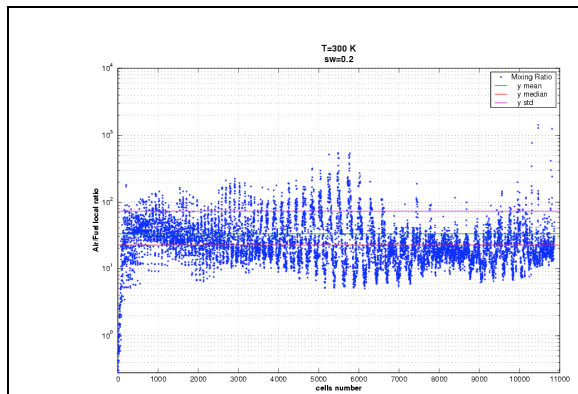
A goal of this work is the determination of concentration profiles varying comburent temperature from 300 up to 1200K. Only the transport has been analysed because liquid fuel combustion is a very hard problem to be modelled due to two-phase flow, with evaporation and coalescence and a big number of chemical reactions.

The shape of the adopted burner is very simple and frequently used.

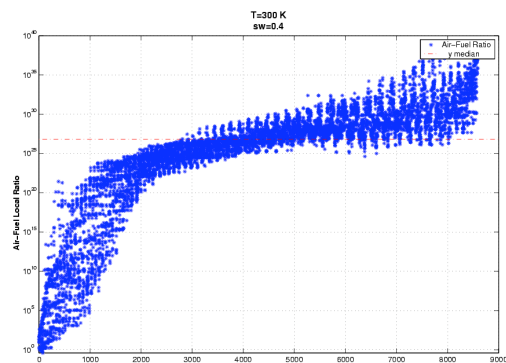
The problem of mass transfer has been modelled considering a number of liquid droplets in a lagrangian domain; this phase consists of spherical particles dispersed in a continuous phase and moved by a swirled jet. The trajectory of the particles together with heat and mass transfer have been calculated, coupling the two phases.

The result of this pre-processing stage has been the determination that the Realizable k- $\epsilon$  model is the most appropriate to simulate this phenomenology: this can be noticed by similarity profiles reported in the following figures.

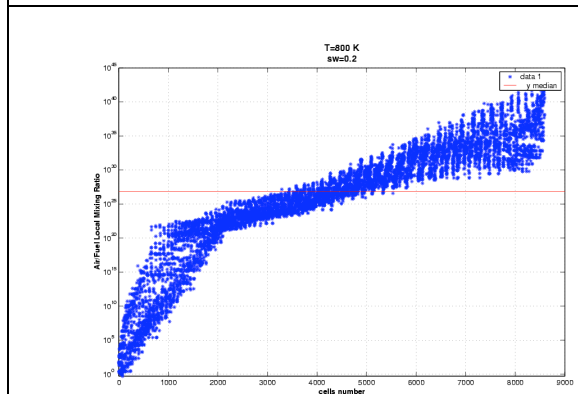
In this condition the diffusion behaviour has been investigated in order to well know the mixing conditions: the diffusion gradient can be demonstrated to be correlated to staying time of fuel droplets in the combustion zone, as described by correlation with turbulent viscosity.



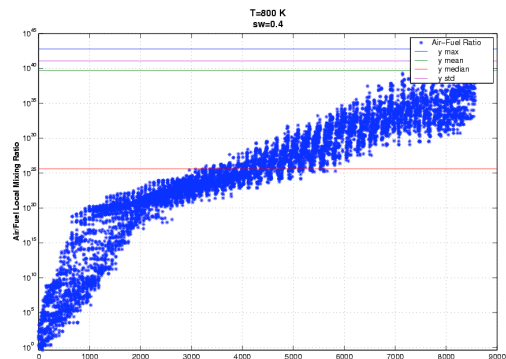
**Fig.2: Air fuel local ratio (T= 300K, SW=0.2)**



**Fig.3: Air fuel local ratio (T= 300K, SW=0.4)**



**Fig.4: Air fuel local ratio (T= 800K, SW=0.2)**



**Fig.5: Air fuel local ratio (T= 800K, SW=0.4)**

In fig. 2,3,4,5, the air-fuel local ratio are reported at two different values of air temperature (300K and 800 K) and swirl number (0.2, 0.4). In these diagram the mean and the maximum values are highlighted together with standard deviation.

In fig. From 6 to 9, the mean and RMS axial velocity are reported, giving the difference between lower and upper air temperature and swirl.

Radial velocity profiles, turbulent viscosity, turbulent kinetic energy and turbulent dissipation have been calculated too, at different distance from the injection section, but not reported for a space matter.

Fuel diffusion coefficients can be analyzed in fig. from 10 to 13, and finally (fig. 14-15) the mean mass fraction profile can be visualized with respect to lower and upper flammable limits of mixture.

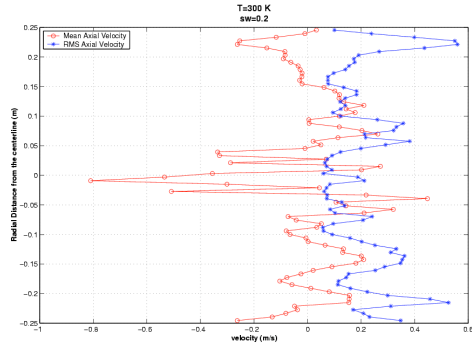


Fig.6: Mean and RMS axial vel. (T=300K, SW=0.2)

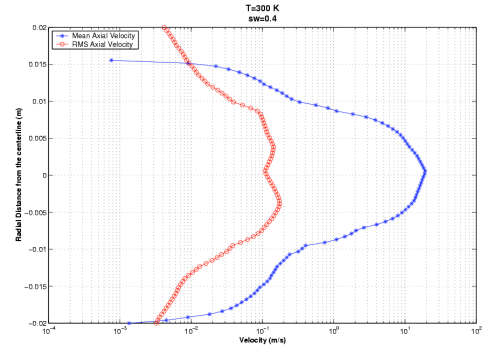


Fig.7: Mean and RMS axial vel. (T=300K, SW=0.4)

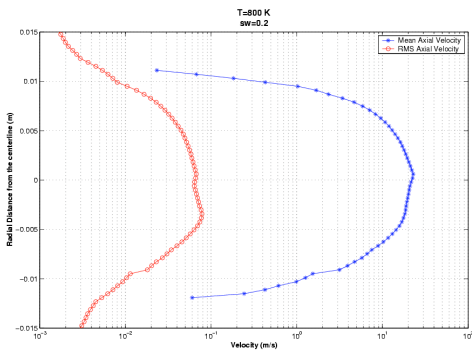


Fig.8: Mean and RMS axial vel. (T=800K, SW=0.2)

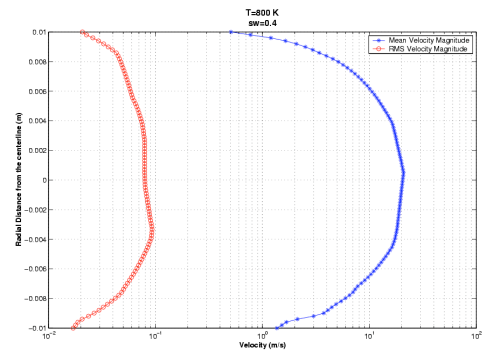


Fig.9: Mean and RMS axial vel. (T=800K, SW=0.4)

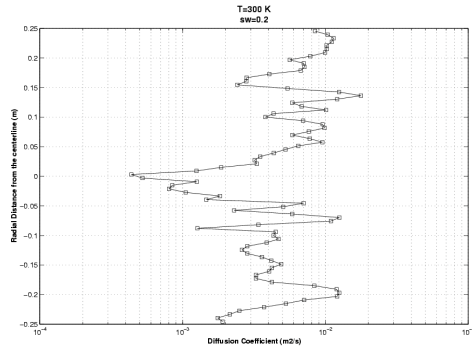


Fig.10: Fuel diffusion coeff. (T=300K, SW=0.2)

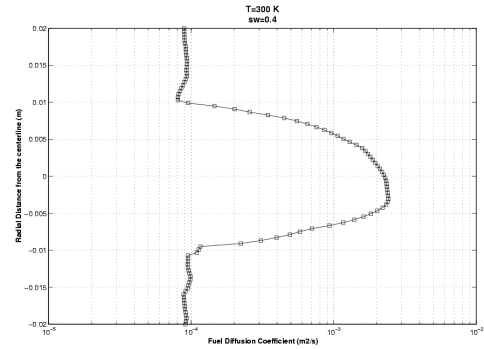


Fig.11: Fuel diffusion coeff. (T=300K, SW=0.4)

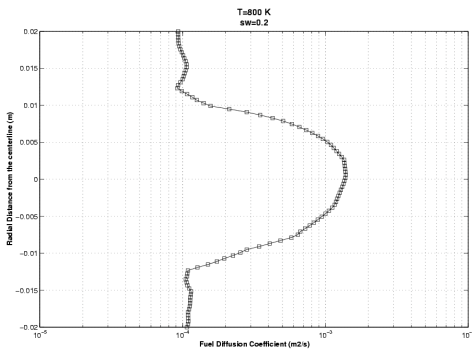


Fig.12: Fuel diffusion coeff. (T=800K, SW=0.2)

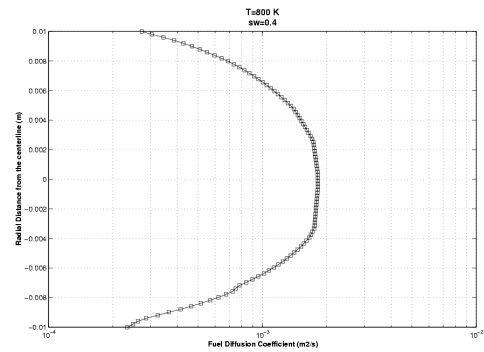
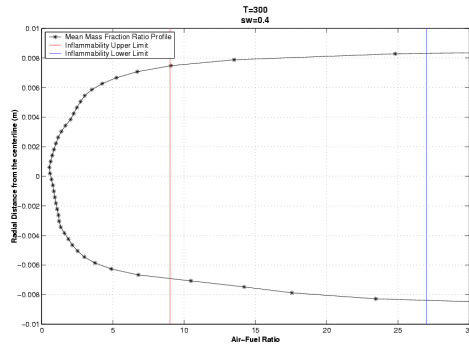
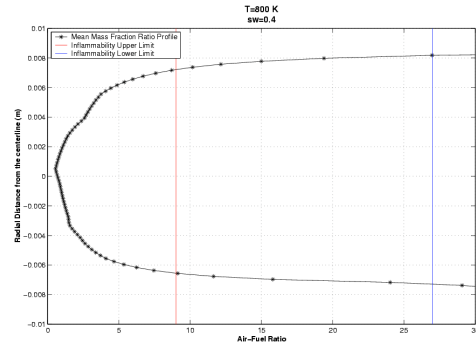


Fig.13: Fuel diffusion coeff. (T=800K, SW=0.4)



**Fig.14: Mean mass fraction ratio profile  
(T=300K. SW=0.4)**



**Fig.15: Mean mass fraction ratio profile  
(T=800K. SW=0.4)**

## 6. Conclusions

It has been investigated about the behaviour of diffusion as a characteristic parameter of mixing conditions: in fact diffusion gradient can be demonstrated to be correlated with the residence time of fuel particles in combustion zone due to the correlation with turbulent viscosity  $\mu_t$ .

The work carried out has highlighted the strong dependence of the system by the injection conditions (swirl and air velocity d temperature).

Next step will be a more accurate study of evaporation and coalescence, up to the simulation of reacting flow in mild combustion conditions. To well simulate this situation a mixture of air and flue gas will be considered and simulated as comburent flow.

## References

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