

# PDF modeling of turbulent combustion of an atomized liquid fuel

F.X. Demoulin<sup>1</sup>, R. Borghi<sup>2</sup>

IRPHE

UMR 6594 CNRS/Université d'Aix-Marseille I et II - ESM2

Technopôle de Château Gombert

13451 Marseille Cédex 20, France

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## Introduction

There are many problems of practical interest where a combustion chamber is fed with a liquid fuel in a turbulent medium, for example, in a car Diesel engine or a direct fuel injection engine. If we assume that the physical characteristics of the spray can be known, the main modeling problem is to build a model for the turbulent combustion, which is able to take into account variable equivalence ratio, diffusion flames and effects due to the spray vaporization.

To represent the state of a burning chemical mixture produced by a mixing of a jet of liquid fuel with a stream of pure air, under the assumptions of a single reaction and equal diffusivities, we need only two chemical variables: the first one, called the mixture fraction, describes the processes of mixing and vaporization, and the second one represents mixing and chemical reaction. Among all possible definitions of the mixture fraction we have chosen here to define:

$$Z(Y_f, Y_{O_2}) = \frac{Y_f - \frac{Y_{O_2}}{\nu} + \frac{(Y_{O_2})_{air}}{\nu}}{1 + \frac{(Y_{O_2})_{air}}{\nu}}, \text{ where } Y_i \text{ is the mass fraction of the species 'i'.} \quad (1)$$

The reactive variable can be simply chosen as the oxidizer mass fraction  $Y_{O_2}$ . In order to compute the mean reaction rate in gas phase, we need the joint probability density function (PDF)  $\tilde{P}(Z, Y_{O_2})$ . Despite the progress of the computer power, it is still difficult to compute this PDF in the practical case even if a Monte-Carlo method is used as it was done by Durand and *al.* [1]. We shall study here the way of presuming a shape of  $\tilde{P}(Z)$ , making an emphasis on the modifications needed to reckon the presence of the spray. If the chemistry is assumed very fast  $\tilde{P}(Z)$  is sufficient in order to compute the whole thermochemical field. In the general case of finite rate chemistry, the joint PDF can be reconstructed from  $\tilde{P}(Z)$  with a model like Modèle Intermittent Lagrangien (MIL) [2].

We shall show a first example of computation, performed using the KIVA code where liquid droplets are represented by lagrangian samples and the gas phase is described with a set of eulerian equations.

## Equation for $\tilde{Z}$ and $\tilde{Z}^2$ including vaporization of droplets

To take into account two phase flows characteristics we use a two fluid flow representation, as in the KIVA code. In this way we obtain two sets of equations, one for the liquid and one for the gas. The mean equations for the two-phase medium are used in the code. But here, we need to write the instantaneous ones, as in [4]. Among this equations there are for the gaseous phase:

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_\alpha}{\partial x_\alpha} &= \rho \omega_v, \\ \frac{\partial \rho Z}{\partial t} + \frac{\partial \rho u_\alpha Z}{\partial x_\alpha} &= \frac{\partial}{\partial x_\alpha} \left( \rho D \frac{\partial Z}{\partial x_\alpha} \right) + \rho \omega_v. \end{aligned}$$

There is a special term in the the mass equation which represents the flux of vapour coming from the evaporation  $\omega_v$ . Because  $\rho$  is the instantaneous gas density, not the mean one, the derivatives must be taken in a generalized sense, since  $\rho$  is discontinuous and vaporization occurs only at the liquid-gas

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<sup>1</sup>e-mail: demoulin@esm2.imt-mrs.fr

<sup>2</sup>e-mail: borghi@esm2.imt-mrs.fr

interface then  $\omega_v$  is proportional to a Dirac  $\delta$ -function. From these exact equations we obtain the equations for  $\tilde{Z}$  and  $\tilde{Z}^2$ :

$$\begin{aligned} \frac{\partial \tilde{\rho} \tilde{Z}}{\partial t} + \frac{\partial \tilde{\rho} \tilde{u}_\alpha \tilde{Z}}{\partial x_\alpha} &= - \frac{\partial \tilde{\rho} \tilde{u}'_\alpha \tilde{Z}'}{\partial x_\alpha} + \frac{\partial}{\partial x_\alpha} \left( \tilde{\rho} D \frac{\partial \tilde{Z}}{\partial x_\alpha} \right) + \tilde{\rho} \tilde{\omega}_v, \\ \frac{\partial \tilde{\rho} \tilde{Z}^2}{\partial t} + \frac{\partial \tilde{\rho} \tilde{u}_\alpha \tilde{Z}^2}{\partial x_\alpha} &= - \frac{\partial \tilde{\rho} \tilde{u}'_\alpha \tilde{Z}'^2}{\partial x_\alpha} + \frac{\partial}{\partial x_\alpha} \left( \tilde{\rho} D \frac{\partial \tilde{Z}^2}{\partial x_\alpha} \right) \\ &\quad - 2 \tilde{\rho} \tilde{u}'_\alpha \tilde{Z}' \frac{\partial \tilde{Z}}{\partial x_\alpha} - 2 \tilde{\rho} D \frac{\partial \tilde{Z}' \partial \tilde{Z}'}{\partial x_\alpha \partial x_\alpha} + 2 \left( \tilde{\rho} \tilde{Z} \tilde{\omega}_v - \tilde{\rho} \tilde{Z}' \tilde{\omega}_v' \right) + \tilde{\rho} \tilde{Z}^2 \tilde{\omega}_v - \tilde{\rho} \tilde{Z}'^2 \tilde{\omega}_v'. \end{aligned}$$

In addition to the usual terms there are extra terms due to the vaporization rate and these terms are unclosed.

Let us introduce  $\phi_s = Z(Y_{f_s}, Y_{O_{2s}})$  the value of  $Z$  at the liquid surface. Using a thermodynamic equilibrium hypothesis and applying the Clapeyron's law,  $Y_{f_s}$  can be expressed as a function of the surface temperature. This value is always lower than unity except when the liquid boils. So, the maximum value of  $Z$  is generally lower than one.  $Y_{O_{2s}}$  takes into account chemistry effects: for instance if chemistry is very fast it is zero.

Assuming that liquid forms a cloud of droplets we can use the generalized 'D-square law' [5] to represent the local rate of evaporation for each droplet. Although  $Y_{O_{2s}}$  and the surface temperature  $T_s$  can vary, we shall assume they keep the same value along the surface of one droplet. Then each droplet has its own value of  $\phi_s$  and there is a PDF for  $\phi_s$  at each location within the flow. Since the vaporization rate is zero everywhere except at the surface, we can express all the correlation with the vaporization rate like:  $\tilde{Z} \tilde{\omega}_v = \phi_s \tilde{\omega}_v = \int \phi_s \omega_v \tilde{P}(\phi_s) d\phi_s$

Because we use Monte-Carlo method to follow the droplets, we are always able to express this integral as a sum over all the stochastic 'k' particles which represent the droplets in the volume  $v$ , thus:

$$\tilde{Z} \tilde{\omega}_v = \sum_k \phi_s^k \left( Y_{f_s}^k(T_s^k), Y_{O_{2s}}^k \right) \frac{\dot{m}^k}{v}, \quad (2)$$

where  $\dot{m}^k$  is the vaporized mass flow rate of the droplet 'k', given by the 'D-square law'. When chemistry is fast  $Y_{O_{2s}}^k = 0$ , in order to introduce finite rate chemistry effects on the conditions at the liquid surface, we could use a lagrangian equation to describe the evolution of  $Y_{O_{2s}}^k$ .

## A PDF with an account for the liquid phase effects

### $Z_{ini}$ — the upper limit of the $Z$ domain for $\tilde{P}(Z)$

An important effect due to the vaporisation is that the upper limit of possible  $Z$  is not known and not unity. This limit can be found looking at the initial value of  $Z$  for a particle issued from the liquid surface, we shall denote it as  $Z_{ini}$ . At the initial moment when the particle is just emitted and it is still at the surface  $Z_{ini} = \phi_s$ . But these quantities are not everywhere the same, since  $\phi_s$  has a meaning only at the liquid surface, whereas  $Z_{ini}$  is defined for any non-zero  $Z$ , even if all the liquid is completely evaporated.  $Z_{ini}$  is a value carried by the fuel vapour as a characteristic of the liquid surface from which the vapour comes. Then the part of the PDF shape for high  $Z$  may be expected to be strongly related to  $Z_{ini}$  and not only to the micro-mixing between the droplets. It is possible to find an equation for  $P_{ini}(Z_{ini})$  as follows. We consider the ratio:

$$\frac{\text{mean of vapour mass evaporated with } Z_{ini} \in [Z_{ini}, Z_{ini} + dZ_{ini}]}{\text{total volume}} = \tilde{\rho} \tilde{Z} P_{ini}(Z_{ini}) dZ_{ini}. \quad (3)$$

We get a balance equation corresponding to this quantity:

$$\frac{\partial \tilde{\rho} \tilde{Z} \tilde{P}_{ini}(Z_{ini}) dZ_{ini}}{\partial t} + \frac{\partial \tilde{\rho} \tilde{u}_\alpha \tilde{Z} \tilde{P}_{ini}(Z_{ini}) dZ_{ini}}{\partial x_\alpha} = \frac{\partial}{\partial x_\alpha} \left( \tilde{\rho} D_t \frac{\partial \tilde{Z} \tilde{P}_{ini}(Z_{ini}) dZ_{ini}}{\partial x_\alpha} \right) + \omega_v|_{Z_{ini}}, \quad (4)$$

where  $\omega_v|_{Z_{ini}}$  is the vaporisation rate conditioned at  $Z_{ini}$ . This equation is in closed form and we can solve it for each point in the  $Z_{ini}$  space. However we will use here only  $\bar{Z}_{ini} = \int Z_{ini} \tilde{P}_{ini}(Z_{ini}) dZ_{ini}$ ,

assuming this quantity is a good approximation on the upper the upper boundary for  $\tilde{P}(Z)$ . We multiply the equation (4) by  $Z_{ini}$  and integrate it along the  $Z_{ini}$  domain to get:

$$\frac{\partial \tilde{\rho} \tilde{Z} \tilde{Z}_{ini}}{\partial t} + \frac{\partial \tilde{\rho} u_\alpha \tilde{Z} \tilde{Z}_{ini}}{\partial x_\alpha} = \frac{\partial}{\partial x_\alpha} \left( \tilde{\rho} D_t \frac{\partial \tilde{Z} \tilde{Z}_{ini}}{\partial x_\alpha} \right) + \int_0^1 Z_{ini} \omega_{v|Z_{ini}} dZ_{ini}. \quad (5)$$

Since the vaporisation is zero every where except at the surface where  $Z_{ini} = \phi_s$ , the last term is equal to the term of equation (2), hence it does not require a special closure.

## A PDF shape based on micro-mixing model

Several kind of PDF shapes are already used, especially a combinations of peaks and rectangles as well as the well-known beta function. These functions were chosen because globally from a geometrical point of view they reproduce qualitatively the essential features of the real PDF. However these shapes do not come from a deduction based on physical considerations, hence it is not straightforward to assess their validity for two-phase flows. We suggest to replace the geometrical consideration by the choice of a PDF shape that would occur in a partially stirred reactor (PaSR) with the residence time distribution given by:

$$P(\tau) = \frac{e^{-\frac{\tau}{t_s}}}{t_s}. \quad (6)$$

Here,  $t_s$  is the mean residence time. We use the lagrangian equation of  $Z$ , coupled with the IEM model [3] to represent the micro-mixing:

$$\frac{dZ}{dt} = \frac{\tilde{Z} - Z}{\tau_Z}. \quad (7)$$

Its integration in a PaSR with initial condition ( $Z = 0, Z = \tilde{Z}_{ini}$ ) leads to an algebraic formulation for the PDF of  $Z$  as a function of  $\tilde{Z}$  and  $\tilde{Z}^2$ :

$$P(Z) = \begin{cases} r \left( 1 - \frac{\tilde{Z}}{\tilde{Z}_{ini}} \right) \frac{(\tilde{Z} - Z)^{r-1}}{\tilde{Z}^r} & \text{if } Z < \tilde{Z}, \\ r \left( \frac{\tilde{Z}}{\tilde{Z}_{ini}} \right) \frac{(Z - \tilde{Z})^{r-1}}{(\tilde{Z}_{ini} - \tilde{Z})^r} & \text{if } \tilde{Z} < Z < \tilde{Z}_{ini}, \\ 0 & \text{otherwise.} \end{cases} \quad (8)$$

where  $\frac{\tilde{Z}^2}{\tilde{Z}(\tilde{Z}_{ini} - \tilde{Z})} = \frac{r}{r+2}$ .

We have drawn on Fig. 1 the PDF shapes for different values of segregation factor  $\left( S_r = \frac{\tilde{Z}^2}{\tilde{Z}(\tilde{Z}_{ini} - \tilde{Z})} \right)$  expressed in percentage. The influence of the value of  $\tilde{Z}_{ini}$  seems to be of the utmost importance. The method used here is quite simple, besides it leads to an algebraic formulation for the mean species mass fractions, henceforth it is very competitive in terms of computer time consumption.

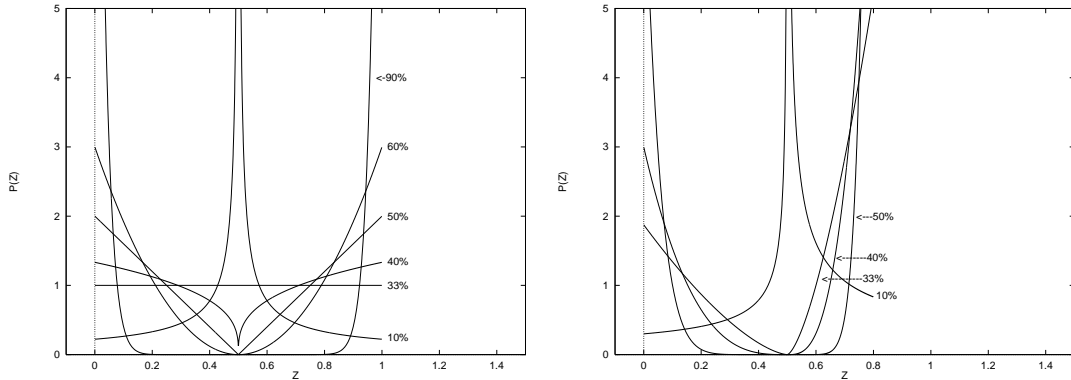


Figure 1:  $P(Z)$  shapes for different values of  $\tilde{Z}_{ini} = 1.0$  (on the right) and  $\tilde{Z}_{ini} = 0.8$  (on the left).

## Application

We test the validity of this procedure by comparison with the experiments of Goix *et al.* [6] for a two-phase flow case. This experiment studies the methanol/air coaxial reacting spray near the stabilization region. The laser-induced fluorescence from OH radical is used as a marker to locate the flame front. The implementation of the  $\tilde{Z}$ ,  $\tilde{Z}^{\prime 2}$ ,  $\bar{Z}_{ini}$  equations in the KIVA code enables us to compute the fields of any interesting thermochemical variable. We have drawn only on Fig. 2 a comparison of an instantaneous measured field of OH with the mean reaction rate obtained with the assumption of infinitely fast chemistry. We represent here the first operating condition from [6], which corresponds to a differential velocity between gas and liquid of about 70m/s. Two reaction zones, one on the center of the jet and the other on the edge of the jet, which are typical for any spray flame are reasonably well reproduced by the modeling. Moreover the position of the flame is at a good agreement with the measurements. This is an important feature, because flame location depends on both evaporation and mixing, which govern also the shape of  $\tilde{P}(Z)$ .

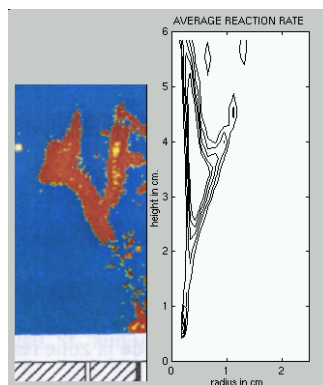


Figure 2: Comparison between the measurement of laser-induced fluorescence from OH radical (on the right) and calculated iso-contours of the mean reaction rate (on the left)

The approach can be generalized to include finite rate chemistry, simply using the MIL model [2]. This will enable us to study situations where the flame is not controlled only by mixing and vaporization.

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