AN EULERIAN MODEL TO IMPROVE THE PRIMARY BREAKUP MODELING OF ATOMIZING JET

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Abstract
This paper addresses the issue of the atomization modeling. In order to take into account the very initial phenomena occurring at the start of this process, the so-called primary break-up, an Eulerian one flow model is used instead of the usual Lagrangian particle models more appropriate for the secondary break-up. In the initial part of the spray the liquid flow is not a set of droplets, and both interactions between liquid-liquid particles and gas-liquid particles are very strong. Due to the high initial velocity difference, between the liquid and the gas flow, the initial mixture flow can be considered as a turbulent flow. Therefore this is the turbulence model that drives the initial dispersion of the liquid. The main point of the work presented here will be a study of what will be an appropriate turbulent model for representing this phenomenon. In order to complete the modeling of the atomization, the whole model includes an equation for the liquid surface density which permits to know a characteristic size of the liquid droplets formed in the end. At the point where the spray is diluted enough, a transition to the Lagrangian particles formulation is initiated in order to benefit of the advantages of this approach in the latest stages of the atomization.

Introduction

The atomization of a liquid jet is classically [1-2] divided in two steps. The first one is the primary breakup, which is occurring usually very close to the nozzle where the spray is very dense. The second one is the secondary breakup, which is occurring after where the spray is diluted. Due to the use of a Lagrangian particle formulation, which is widely spread to describe the liquid phase, most of the models are making the assumption that the liquid is a set of droplets, even in the liquid core of the jet ("Blob" hypothesis). The sizes of those liquid parcels are initialized with an empirical law depending on the diameter of the injector. Eventually models based on linear instabilities [3-4] are used to represent the breakup of those droplets and then their size evolution. Those approaches where the liquid phase is always represented by a set of droplets seems very appropriate for the secondary breakup. The extension of the validity of those approaches for the primary breakup where a liquid core can exist is more questionable. We believe that this is a key point, which needs to be improved in order to get a better representation of the atomization.

Close to the injector nozzle, the liquid volume fraction is sufficiently high to expect strong interactions between the liquid phase itself. At the tip of the injector, usually a high velocity gradient exists which leads to a large level of turbulence therefore a two phase turbulent jet is produced, which produces the liquid dispersion. Before this, inside the injector, the cavitation can help the breakup of the liquid phase as shown in several studies [5]. It is probably not enough to represent this phenomenon by only the reduction of the effective diameter of the injector: velocity fluctuations and of the liquid volume fraction must be taken into account. Technically, it's well known that to get good results for the liquid penetration for example, the size of the mesh close to the injector must be of the same order as the injector nozzle [6]. So, it's necessary to have a method able to manage mesh cells completely filled by liquid and where the used hypothesis that the liquid volume must be negligible compared to the volume of the mesh cell is not acceptable.

All these phenomena are important, they must be taken into account during the primary breakup and their implementation in a Lagrangian particle method seem not easy. Another and more attractive alternative is to use an Eulerian method. This new approach is considered here and leads to a model appropriate for the first step of the atomization, theoretically this model can be used also for the entire atomization phenomenon. However, because of the Lagrangian particles method advantages when the spray is diluted, it is appealing to link together both methods.

Overview of the model

The model described originally in [7] consists on a one flow Eulerian representation of the liquid/gas mixture closed to the nozzle of the injector. Equations for the mean velocity of the two phase flow and for the mean liquid mass fraction are used to describe this flow, average and fluctuations are taken using mass weighted Favre average. For Weber and Reynolds number "high" enough the initial breakup and dispersion of the liquid is only due to the turbulent mixing between the gas and the liquid. Therefore, only an appropriate turbulent model, able to manage flow with very high density ratio, is necessary to describe the evolution of the liquid mass fraction in this zone. However, to know the size of the droplets, which are the smallest scales of the liquid parcels, we have to consider that the surface tension acts sufficiently to prevent any further breakup. Assuming that the size of the liquid parcels

is always given by an equilibrium between the surface tension forces and the inertia forces, a critical Weber number permits to estimate the mean radius of the droplets. But this hypothesis is too restrictive, and in order to avoid it, a transport equation for the mean liquid surface density $\overline{\Sigma}$ is considered. The Sauter mean diameter of the liquid parcels is then proportional to the ratio $\widetilde{Y}_l / \overline{\Sigma}$. The exact equation for the mean liquid surface density could be derived but it would be too difficult to consider of each terms therefore a postulated equation will be used as for the transport equation of the flame surface density in the field of turbulent combustion, details of this equation can be found in [7].

The turbulence model must be revisited to check its ability to reproduce the initial dispersion of the liquid. In this work we will focus our attention on this point of the whole model. To achieve this goal we will consider a second order closure using equations for the Reynolds stress tensor and for the liquid turbulent flux $\widetilde{u"_i Y_l}$. The exact equation derived for these quantities contains terms relative to the density variation. These terms are usually neglected for gas-gas flow with low density variation (density ratio lower than ten). For separated flow (the liquid does not diffuse in the gas) these terms are shown to be proportional to $\overline{\rho}(1/\rho_l - 1/\rho_g)$. Therefore for high density ratio, as those encounter in a liquid–gas mixture, these terms must be taken into account. The usual closure for all the other terms has to be examined to determine whether or not it is still valid.

Finally it is interesting to consider the coupling between Eulerian and Lagrangian approaches. To get both the advantages of the Eulerian formulation inside the dense part of the spray and of the Lagrangian one inside the diluted region of the spray, it is necessary to link together both approaches. In order to switch to the Lagrangian formulation a criteria is introduced. The new created numerical particles representative of the spray have to be initiated, on this purpose, a method to extract the liquid velocity and the liquid turbulence intensity from their corresponding variable for the liquid/gas mixture flow in the Eulerian representation is developed [8]

Description of the initial dispersion of the liquid using a turbulence model

We assume that the liquid and the gas close to the injector interact together as a unique flow but containing two species. Since there is a huge differential of velocity between the gas and the liquid , typically Δu is of the order of 100 m/s, it can be expected that the mixing layer, which is developed from the initial interface, is turbulent. Therefore one can use a kind of k-epsilon model applied to the two-phase turbulent flow to describe this zone. Here we try such models but also we are interested on a second order approach because it carries much more indications on what can be the effect of the high density ratio that characterises such liquid-gas flows.

The equation for the turbulent kinetic energy, or more generally, the equations for Reynolds stress tensor can even be derived taken into account density fluctuation. The $\overline{u_i^{"} u_j^{"}} - \varepsilon$ equations are expected to be more sensitive to the terms related to the compressible effects in this case and even those neglected in low variable density cases. The equations can be derived as follows:

$$\frac{\partial \overline{\rho} R_{ij}}{\partial t} + \frac{\partial \overline{\rho} R_{ij} \tilde{U}_k}{\partial x_k} = P_{ij} + D_{ij} + \Phi^c{}_{ij} + C_{ij} - \overline{\rho \varepsilon_{ij}} \tag{1}$$

$$D_{ij} + P_{ij} = -\frac{\partial}{\partial x_k}\left(\overline{\rho} \widetilde{u_i^{"} u_j^{"} u_k^{"}} + \overline{p' u_i^{"}} \delta_{jk} + \overline{p' u_j^{"}} \delta_{ik} \right) - \overline{\rho} \widetilde{u_i^{"} u_k^{"}} \frac{\partial \widetilde{u_j}}{\partial x_k} - \overline{\rho} \widetilde{u_j^{"} u_k^{"}} \frac{\partial \widetilde{u_i}}{\partial x_k} \tag{2}$$

$$C_{ij} = \left(\overline{u_j^{"}} \frac{\partial \overline{P}}{\partial x_i} + \overline{u_i^{"}} \frac{\partial \overline{P}}{\partial x_j} \right), \overline{u_i^{"}} = \overline{\rho}\left(1/\rho_l - 1/\rho_g\right) \widetilde{u_i^{"} Y_l^{"}} \tag{3}$$

$$\Phi_{ij}^c = \Phi_{ij} + \gamma' \left(\overline{u_i^{"}} \frac{\partial \overline{P}}{\partial x_j} + \overline{u_j^{"}} \frac{\partial \overline{P}}{\partial x_i} - \frac{2}{3} \overline{u_k^{"}} \frac{\partial \overline{P}}{\partial x_k} \delta_{ij} \right) \tag{4}$$

Where R_{ij} represents the Reynolds Stress Tensor, P_{ij} the production terms, D_{ij} the diffusion term, Φ_{ij}^c the redistribution term and C_{ij} the compressible term. The effect of molecular viscosity is neglected here since we assumed a high Reynolds number. The C_{ij} term is often negligible, but for separated flow (the liquid does not diffuse to the surrounded gas), $\overline{u_i^{"}}$ can be expressed exactly, and is proportional to the density ratio. Therefore, this term can be important for large enough density ratios, which must be taken into account. As for the other classical production terms, a contribution proportional to C_{ij} is added to the model, more precisely to the redistribution term with a constant γ'=0.75 [7]. The contribution of these terms to the equation for $\tilde{\varepsilon}$ is included in a standard manner [7].

A second order closure for the turbulent flux of the liquid $\widetilde{u_i^{"} y^{"}}$ is considered . The exact equation is derived as follows:

$$\frac{\partial}{\partial t}\left(\overline{\rho u_i'' y''}\right)+\frac{\partial}{\partial x_j}\left(\overline{\rho u_i'' y''}\tilde{U}_j\right)=-\frac{\partial}{\partial x_j}\left(\overline{\rho u_i'' u_j'' y''}+\overline{p' y''}\delta_{ij}\right)-\overline{\rho u_i'' u_j''}\frac{\partial \tilde{Y}}{\partial x_j}-\overline{\rho u_j'' y''}\frac{\partial \tilde{U}_i}{\partial x_j}$$
$$-\overline{y''}\frac{\partial \overline{P}}{\partial x_i}+\overline{p'\frac{\partial y''}{\partial x_i}} \qquad (5)$$

The last two terms are possible sources of density variation effects, the first one is obtained exactly and the second one is closed in classical manner [9-10], but incorporating the effect of the first term [7]:

$$\overline{y''}\frac{\partial \overline{P}}{\partial x_i}=\overline{\rho}\widetilde{Y}_l(1-\widetilde{Y}_l)\left(1/\rho_l-1/\rho_g\right)\frac{\partial \overline{P}}{\partial x_i} \qquad (6)$$

$$\overline{p'\frac{\partial y''}{\partial x_i}}=-\alpha\,\overline{\rho u_i'' y''}\frac{\tilde{\varepsilon}}{\tilde{k}}+\beta\,\overline{\rho u_j'' y''}\frac{\partial \tilde{u}_i}{\partial x_j}+\gamma_y\,\overline{y''}\frac{\partial \overline{P}}{\partial x_i} \qquad (7)$$

The first three terms attached to the constants α,β,γ_y are the usual terms used to described a mixture with a low density ratio [11-12], here we take $\alpha=5,\beta=0.5,\gamma_y=0.5$ as in [7,13] .

Test of the model on co-axial injector

The model is tested on the configuration corresponding to a co-axial injector. These kind of injectors are composed of a slow centered liquid jet surrounded by a high velocity jet of gas. For example this injector can be encountered in rocket engine. The experiment, used as test case, used water and air as liquid and gas fluids. The schematic of the injector is presented on figure 1:

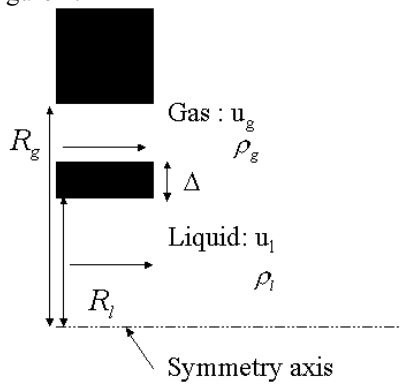

Figure 1. Schematic of the injector

The model is incorporated in a parabolic code based on the hypothesis that the flow has the characteristic of a mixing layer. This is of interest because of the code simplicity, the rapidity of the run and also there is a difficulty due to the presence of an incompressible flow, the water, together with a compressible flow, the gas. The drawback is that it is not possible to take into account explicitly the recirculation induced by the gap of thickness Δ between the liquid jet and the air jet. Basically this thickness is ignored in the present result, but its influence was studied by testing different turbulent input conditions. Based on this tests, the influence of this geometrical simplification is not important for the cases presented here.

The first experiment presents the evolution of the volume fraction along the symmetry axis. The measurement in the dense region of the spray is a difficult task, the fluorescence of an added substance incorporated in the water by a laser sheet is used here [14]. The characteristics of the experiment are R_g=1.7mm, R_l= 0.9mm, Δ=0.25mm, u_g=115m/s, ρ_g =1.2kg/m3, u_l=1.3m/s, ρ_l =1000kg/m3 .

The result of the model presented figure 2. are quite bad in comparison to the experimental data both using k-ε model (referenced as 1st order closure) or second order model (referenced as 2nd order closure). Using the k-ε model but increasing the turbulent diffusion by changing the turbulent Prandt number one can obtain a better result (referenced as increased 1/Prandt Nb), but still different from the measuring data. It could be an effect of the approximations done by using a parabolic code, but it seems more likely that some part of the model must be revisited.

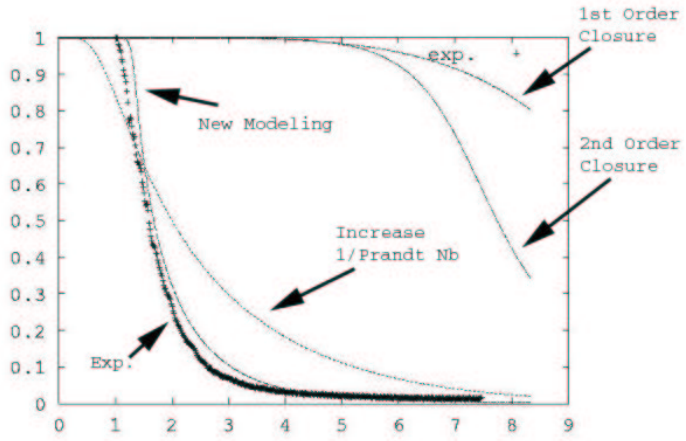

Figure 2. Liquid volume fraction on the injection axis. Experimental results vs. different modeling approaches

Based on DNS type computations of a mixing layer between two fluids of density ratio up to 40, done by Silvani [15], one can find a dependence of the turbulent Prandt number on the local density ratio $1/\mathrm{Pr}_t \propto 1+(\overline{\rho}/\rho_g - \overline{\rho}/\rho_l)$. A new insight of the model at the light of this clue permits to propose a modification of the model as follow. For flow with density stratification the gravity can act as a destabilizing or stabilizing force, this phenomenon was model by Lumley [16] and Launder [17-18] by adding a new contribution in the equation of the turbulent flux due to the correlation $\overline{p' y''_{,i}}$:

$$\overline{p'\frac{\partial y''}{\partial x_i}} = \ldots + C_{y3}\overline{\rho}(1/\rho_l - 1/\rho_g)\overline{\rho Y_l'' Y_l''}\ \ g_i \text{, where } C_{y3} = 1/3. \tag{8}$$

For the destabilizing case, this term expresses the increase of turbulent mass flux due to phenomena linked to Raleigh-Taylor instability. It can also represent the baroclinic effect on secondary instability of a variable density mixing layer [19]. In our case, we also have density stratification but we don't take into account the gravity assuming an high Froud number. Still the flow is accelerated randomly by the fluctuating acceleration induced by turbulent motions. The turbulent acceleration can be taken proportional to the turbulent kinetic energy divided by a characteristic length scale. If we chose that length scale as the inverse of the mean scalar gradient we obtained:

$$\overline{p'\frac{\partial y''}{\partial x_i}} = \ldots + C_{yr}\overline{\rho}(1/\rho_l - 1/\rho_g)\overline{\rho}k\frac{\partial \tilde{Y}_l}{\partial x_i} \tag{9}$$

This modification in the second order closure can lead to a modification for the first order closure by assuming that we reach an equilibrium in order that the turbulent flux is obtained as a balance between the dissipation term, the classical production term in equation (5) and the added term (9), thus:

$$\begin{aligned} &-\overline{\rho u_i'' u_j''}\frac{\partial \tilde{Y}}{\partial x_j} - \alpha\,\overline{\rho u_i'' y''}\frac{\tilde{\varepsilon}}{\tilde{k}} + C_{yr}\overline{\rho}(1/\rho_l - 1/\rho_g)\overline{\rho}k\frac{\partial \tilde{Y}_l}{\partial x_i} \simeq 0 \\ &\Rightarrow -\overline{\rho u_i'' y''} \simeq \overline{\rho}\left(\underbrace{\frac{\widetilde{u_i'' u_j''}k}{\alpha\varepsilon}}_{D_t} + \frac{C_{yr}k^2}{\alpha\varepsilon}\overline{\rho}(1/\rho_g - 1/\rho_l)\right)\frac{\partial \tilde{Y}}{\partial x_j} \end{aligned} \tag{10}$$

The first term in the parentheses corresponds to model the turbulent mass flux using a gradient hypothesis and turbulent diffusion, D_t. The second term is a correction acting only for high density ratio similar to those indicated by result in [15]. Adjusting the constant in order that the ratio C_{yr}/α =2.5 leads to the result referenced on figure 2 as "new modelling".

This approach seems coherent and it permits to fit the computational result with the experimental results. In order to clarify wether or not this explanation is valid we work on a more extended validation. For instance the model is tested against another experimental apparatus but still on a co-axial injector but with different geometrical and velocity input characteristics. The Liquid Presence Probability (LPP) along the axis of the injector is measured using a optic fibre as phase sensor for the liquid phase, see [20-23]. Although it is not clear that the measured LPP is really the volume fraction of the liquid, both are probably very close when LPP>50%. The characteristics of the experiment are R_g=1.8mm, R_l= 1.05mm, Δ=0.20mm, u_g=175m/s, ρ_g =1.2kg/m3, u_l=2.5m/s(exp.1) or u_l=5.0m/s (exp.2), ρ_l =1000kg/m3 .

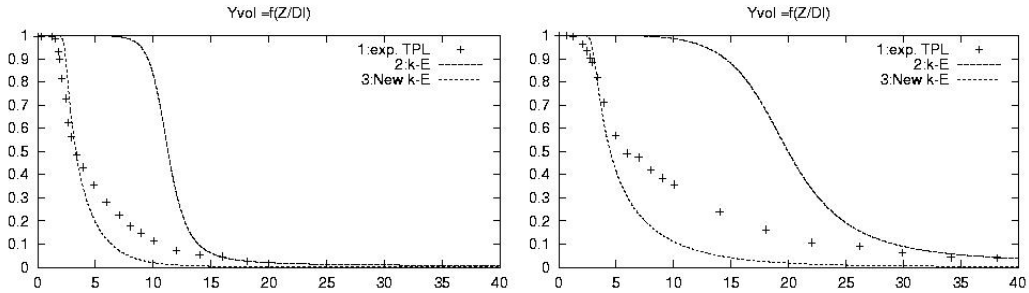

Figure 3. Comparison of the Liquid Probability Presence, (1), with the result obtain with the classical k-ε model, (2), and the modified k-ε model (3) for ul=2.5m/s (left) and ul=0.5m/s (right).

Presented on figure 3 are the results obtain with the original k-ε model and the modified model. The comparison show that the modification discussed above improve the model prediction. Other test are planned in order to test the modified k-ε model extensively. In particular we are trying to implement this model on usual 3D codes that are able to take into account the thickness of the solid boundary between the two jets.

Effect of the turbulence model on the whole atomisation process

The modifications of the mixing turbulent model are implemented in KIVA II and used in conjunction with the new Eulerian atomisation model. The test case presented below is typical of Diesel injection with an injector hole diameter of 200 microns. The velocity injection profile is about 220m/s at 0.11ms after the start of injection. Figure 4 shows the effect of the turbulent mixing model modifications on the liquid volume fraction distribution. The modification leads to shorter length of the so called "liquid core". The shape of the liquid jet stays globally the same. We can just notice a small increase in the spray angle which may be due to the increase of the mixing process generated by the modification. Thanks to the equation for the density of liquid surface it is possible to find a characteristic size of the liquid droplets produced [7]. Figure 5 presents the mean equivalent radius distribution with and without the turbulent mixing model modifications. With the modification we can notice an increase of the number of equivalent droplets and a modification of the shape of the distribution.

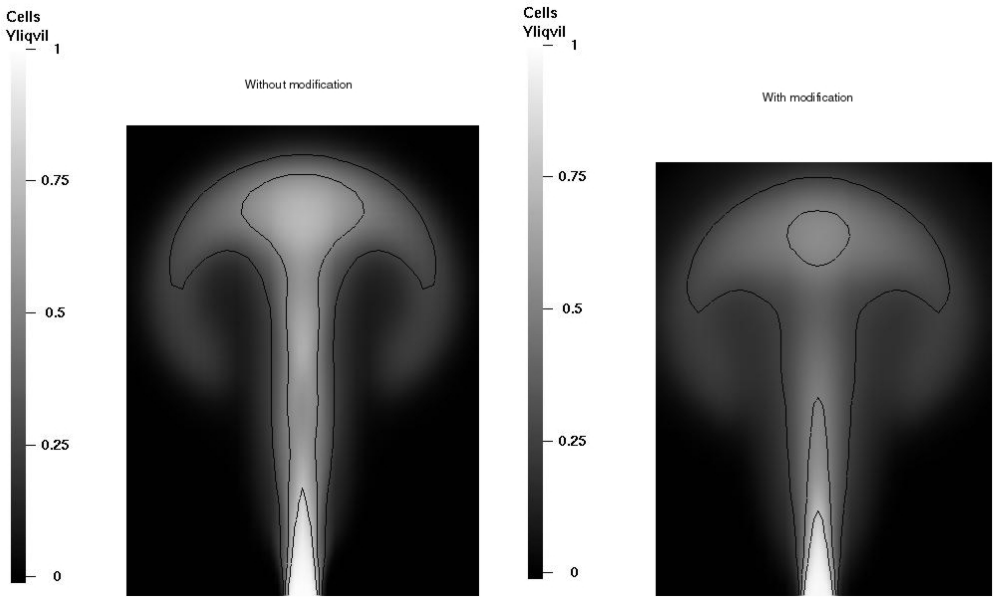

Figure 4. Influence of the turbulent mixing model modification on the liquid volume fraction (without modification on the left, with modification on the right)

Conclusions and perspectives

In the context of a complete atomisation model including the primary break-up, a model for the turbulent mixing is necessary to describe the initial dispersion of the liquid in the liquid-gas mixture. Comparisons with experiments on co-axial injector using a parabolic code show a necessary modification of classical models. A physical model trying to describe the increase in turbulent flux due to Raleigh-Taylor instability is proposed. First tests of this modification are performed and its influence on the complete model is shown. Further works and test are still needed either to validate this modification or to propose an other answer.

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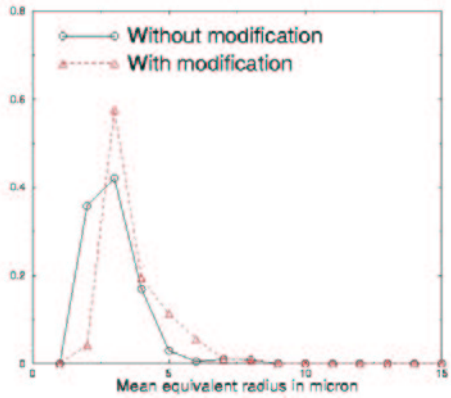

Figure 5. Influence of the turbulent model modification on the global mean equivalent radius distribution

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