AN EULERIAN APPROACH FOR SPRAY MODELLING IN INTERNAL COMBUSTION ENGINES

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ABSTRACT

This paper describes an Eulerian model developed to simulate two-phase flows in internal combustion engines. This model is based on a two-fluid-two-pressure approach that solves a system of transport equations for each phase: liquid fuel (i.e. spray) and gas (fuel vapour and air). Closures adopted for interfacial exchange source terms between the two phases are also presented. These closures assume a spherical droplets hypothesis as a first approach that should be considered in the future. Turbulent effects are not accounted for in this work. The Eulerian model, implemented into the IFP code IFP-C3D, is then validated through several tests. These tests allow to check both the implementation of the liquid phase transport equations and the source terms closures. Finally, a 2D injection-evaporation test is presented as a first step towards real engine applications.

1 - INTRODUCTION

The development of direct injection strategies of liquid fuel in internal combustion engines requires an accurate prediction of physical phenomena related to sprays (injection, evaporation, …). The Lagrangian approach usually employed to compute these phenomena encounters severe shortcomings. This is due to the fact that direct injection systems lead to dense sprays, especially close to the nozzle, whereas the Lagrangian approach is based on a dispersed sprays hypothesis. An Eulerian model is thus desirable to ensure a correct spray modelling for both high and low liquid volume fractions (i.e. near and far from the nozzle).

Eulerian models found in the literature can be classified into two main categories:

- Locally homogeneous models (see for example [1-3]) consider liquid fuel and gaseous phase (i.e. fuel vapour plus air) as a mixture for which only one system of transport equations is solved. An equation of state, that allows to describe both gaseous and liquid phases, represents one of the major difficulties of this kind of model.
- Two-fluid models (see for example [4-6] or [7] for multi-fluid models) consider each phase separately and consequently solve a system of transport equations for each of the two phases. Although this kind of model provides quantities (like velocity) for each phase (i.e. that it does not need an additional model to compute the relative velocity between liquid and gaseous phases as for locally homogeneous models), it is characterised by a main difficulty related to the unclosed interfacial source terms of mass, momentum and energy exchanges between liquid and gaseous phases in the transport equations.

To capture the high velocity difference and temperature gradient at the exit of the nozzle (especially in direct injection Diesel engines), we choose a two-fluid model. It comprises seven transport equations (continuity, momentum and specific internal energy for each phase plus a transport equation for the liquid volume fraction). Since our goal is to develop a model that allows to simulate both dense and dispersed sprays, it is necessary to adopt a two-pressure model that computes both liquid and gaseous pressures [8] and not assumes an equilibrium hypothesis, which considers that liquid pressure is equal to the pressure in the surrounding gas, as in [7,9,10].

In this paper a brief description of the two-fluid-two-pressure model we adopt to simulate two-phase flows in internal combustion engines is given. This model will be presented along with closures we use for interfacial exchange source terms between the two phases. Then several validation test cases will be presented. Some of these tests are devoted to validate the implementation of the liquid phase transport equations and the others aim at evaluating the closures adopted for the interfacial source terms between the two phases. Finally results of a 2D preliminary test, that represents the injection-evaporation of a spray inside a hot vessel, will be briefly discussed. This test represents a first step towards engine applications with our model.

2 - TWO-FLUID-TWO-PRESSURE MODEL

Eulerian approaches are based on distinguishing liquid and gaseous phases inside each control volume V (typically equal to the volume of a cell of the 3D computational grid). To this purpose, liquid, α_l, and gas, α_g, volume fractions are used. The first quantity is computed by solving a transport equation:

$$\frac{\partial \alpha_l}{\partial t} + U_{l,i}\frac{\partial \alpha_l}{\partial x_i} = \frac{\Gamma_l}{\rho_l} \tag{1}$$

where $U_{l,i}$ is the i-component of the liquid velocity and Γ_l the source term due to evaporation of the liquid fuel. The gaseous volume fraction, α_g, which represents the volumic proportion of the fuel vapour and all species contained in the air, can be deduced from:

$$\alpha_g + \alpha_l = 1 \tag{2}$$

The transport equation (1) of the liquid volume fraction, α_l, is coupled with the Navier Stokes equations written below:

$$\frac{\partial \alpha_k \rho_k}{\partial t} + \frac{\partial \alpha_k \rho_k U_{k,i}}{\partial x_i} = \Gamma_k \tag{3}$$

$$\frac{\partial \alpha_k \rho_k U_{k,i}}{\partial t} + \frac{\partial \alpha_k \rho_k U_{k,i} U_{k,j}}{\partial x_j} = -\alpha_k \frac{\partial P_k}{\partial x_i} + \frac{\partial}{\partial x_j}(\alpha_k \tau_{k,ij}) + \alpha_k \rho_k g_i + M_{k,i} \tag{4}$$

$$\frac{\partial \alpha_k \rho_k e_k}{\partial t} + \frac{\partial \alpha_k \rho_k e_k U_{k,i}}{\partial x_i} = -\frac{\partial \alpha_k q_k}{\partial x_i} - \alpha_k P_k \frac{\partial U_{k,i}}{\partial x_i} + \tau_{k,ij}\frac{\partial \alpha_k U_{k,i}}{\partial x_i} + E_k \tag{5}$$

where the subscript k represents the phase ($k=l$ for the liquid phase and $k=g$ for the gaseous one). Note that these equations have been derived following a RANS (Reynolds Averaged Navier Stokes) approach. Mean symbols have been omitted to simplify the presentation of the model. Turbulent effects are not accounted for and will be the subject of a future paper. Pressure, P_g, in the gaseous phase is obtained from the perfect gas equation of state. To compute the pressure, P_l, in the liquid phase we do not assume an equilibrium hypothesis that allows to consider this pressure is equal to P_g but we use the stiffened gas equation of state [11]:

$$P_l + P_\infty = (\gamma - 1)\rho_l C_{V,l} T_l \tag{6}$$

Mass, momentum and internal energy source terms, that appear in eqs (3) to (5), write:

$$\Gamma_k = \rho_k(U_{I,i} - U_{k,i})n_{k,i}\delta_I \tag{7}$$

$$M_{k,i} = (\rho_k U_{k,i}(U_{I,j} - U_{k,j}) + \tau_{k,ij})n_{k,j}\delta_I \tag{8}$$

$$E_k = (\rho_k e_k(U_{I,i} - U_{k,i}) - q_{k,i} + \tau_{k,ij}V_{k,i})n_{k,i}\delta_I \tag{9}$$

where $n_{k,i}$ is the i-component of the unit normal to the interface going out of phase k and δ_I a Dirac distribution attached to the interface. As can be noticed, the momentum source term, M_k, contains two contributions: momentum exchange resulting from mass exchange between liquid and gaseous phases, and viscous effects at interfaces. In the same way, the internal energy source term, E_k, contains three contributions: energy exchange resulting from mass transfer, viscous friction and heat transfer. Following [5,12,13], a spherical droplets hypothesis is adopted as a first approach to close these source terms:

$$\Gamma_l = -\Gamma_g = -\alpha_l \frac{6}{d^2}[\rho D]Sh\ln(1 + B_M) \tag{10}$$

$$M_{l,i} = \Gamma_l V_{l,i} - F_{d,i} \quad ; \quad M_{g,i} = \Gamma_g V_{g,i} + F_{d,i} \tag{11}$$

$$E_l = \Gamma_l e_I + \left|F_{d,i}U_{l,i}\right| - \alpha_l \frac{6}{d^2}\lambda_g Nu \frac{\ln(1 + B_M)}{B_M}(T_l - T_g) \tag{12}$$

$$E_g = \Gamma_g e_I + \left|F_{d,i}U_{g,i}\right| + \alpha_l \frac{6}{d^2}\lambda_g Nu \frac{\ln(1 + B_M)}{B_M}(T_l - T_g) \tag{13}$$

where $F_{d,i}$ is the drag force modeled as in [5] and d a characteristic droplet diameter. It is deduced from the local liquid volume $V_l = \alpha_l V$, and the local droplets number N:

$$d = \sqrt[3]{\frac{6\alpha_l V}{N\pi}}, \tag{14}$$

N is obtained by solving the transport equation:

$$\frac{\partial N}{\partial t} + U_{l,i}\frac{\partial N}{\partial x_i} = 0 \tag{15}$$

Note that coalescence and break-up phenomena are not accounted for. Quantities used in the equations of the model are defined in the nomenclature.

3 - ANALYTICAL VALIDATIONS

The two-fluid-two-pressure model presented in the previous section has been implemented into IFP-C3D code [14]. This parallel code is developed at IFP to simulate two-phase reactive flows in internal combustion engines. It uses an ALE (Arbitrary Lagrangian Eulerian) method to compute these flows on moving unstructured hexahedral grids following a RANS approach. The original version of the IFP-C3D code uses a Lagrangian approach for spray modelling. The Eulerian model has been implemented in parallel with Lagrangian one in such a way to have both approaches available in the code.

First monophasic tests have been achieved in order to check the implementation of the liquid phase equations. In these tests, only liquid phase is considered. It means that $\alpha_l=1$ and $\alpha_g=0$. In the following, two of these tests are presented.

The first test corresponds to a Poiseuille flow in a 2D channel with one inlet (left boundary) and one outlet (right boundary) linked by no-slipping walls (top and bottom boundaries). The analytical velocity solution is imposed at the inlet and a given pressure is fixed at the outlet. Starting from a null velocity field in the channel, the solution converges after 110000 iterations to the results presented in figures 1 and 2. As can be observed, the pressure gradient between the inlet and the outlet is established giving a constant pressure gradient that compares very correctly with the analytical solution (see figure 1). The velocity profile has also been established in all the channel as can be observed in figure 2. The slight difference that can be observed between numerical and analytical solution is due to the fact that the numerical solution is not entirely converged (i.e. that it needs much longer CPU time to obtain a perfectly converged solution).
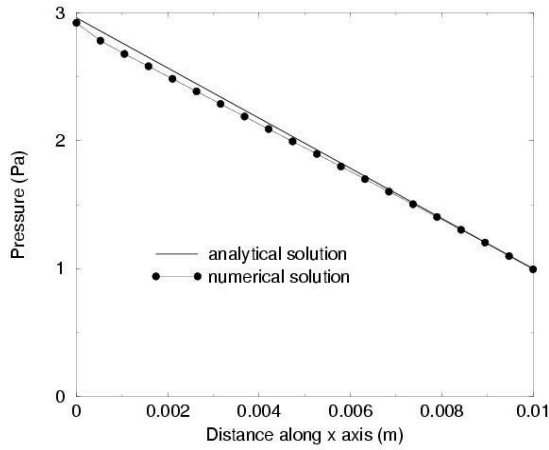
Figure 1: Pressure profile along the channel
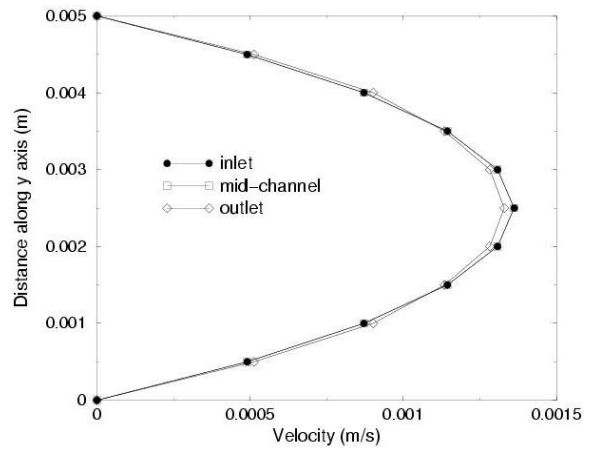for the Poiseuille flow test.

Figure 2: Velocity profiles for the
Poiseuille flow test.

The second test represents the decay of a viscous Green-Taylor vortex [15]. A 2D geometry, on which the following analytical solution is initialised, is used :

$$V_{l,x}(x,y,t) = \sin(\frac{\pi x}{L})\cos(\frac{\pi y}{L})F(t) \tag{16}$$

$$V_{l,y}(x,y,t) = -\cos(\frac{\pi x}{L})\sin(\frac{\pi y}{L})F(t) \tag{17}$$

$$P_l(x,y,t) = P_0 + \frac{\rho_l}{4}(\cos(2\frac{\pi x}{L}) + \cos(2\frac{\pi y}{L}))F(t)^2 \tag{18}$$

where $F(t) = e^{-2\frac{\pi^2 \mu_l t}{\rho_l L^2}}$ and L is the length of the square side. Figures 3 and 4 present respectively velocity and pressure profiles in the diagonal direction of the mesh at different instants. These two figures show that numerical and analytical solutions are superposed and consequently the decay of the vortex is well predicted.

A second category of tests has been performed in order to evaluate source terms Γ_k, M_k, E_k, in eqs (3) to (5) that quantify interfacial exchanges between liquid and gaseous phases. In this paper two tests are presented. The first one is devoted to momentum exchange (source term M_k). A homogeneous distribution of moving droplets is initialised in a motionless gas in a 3D channel with periodic boundaries in the direction of the flow. Relative velocity,U_r, between gas and droplets have to decrease following the analytical solution: $U_r(t) = U_0 e^{-kt}$ with $k = \frac{18\mu_g}{\rho_l d^2} + \frac{18\alpha_l \mu_g}{\alpha_g \rho_g d^2}$ and where U_0 is the liquid initial velocity. Several distributions of moving droplets have been tested, as can be observed in figures 5 and

6 which compare analytical and numerical solutions for $\alpha_l{=}0.05$ and $\alpha_l{=}0.5$ respectively. IFP-C3D reproduces rigorously the analytical decrease of the relative velocity in both cases.
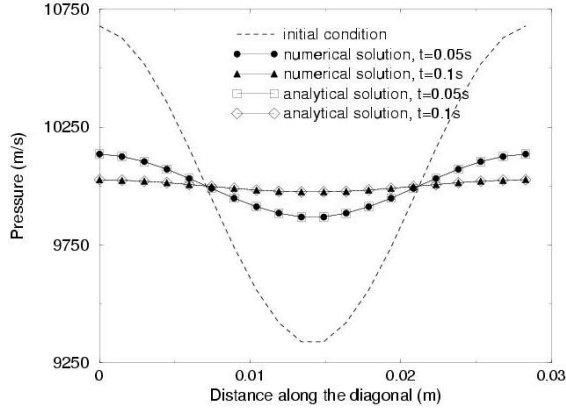

Figure 3: Decay of the Green-Taylor vortex: pressure profile along the diagonal of the mesh at different instants.
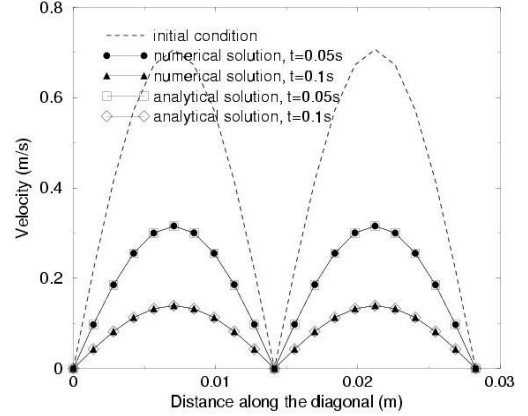

Figure 4: Decay of the Green-Taylor vortex: velocity profiles along the diagonal of the mesh at different instants.
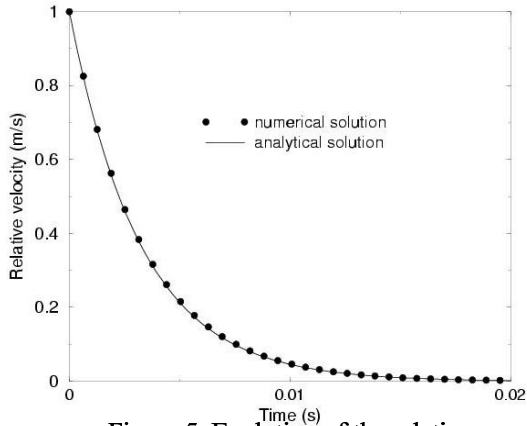

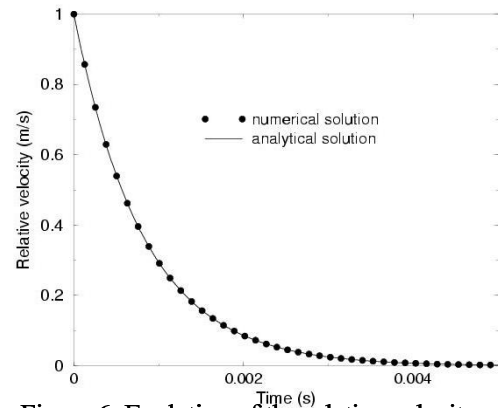Figure 5: Evolution of the relative velocity for $\alpha_l = 0.05$.

Figure 6: Evolution of the relative velocity for $\alpha_l = 0.5$.

The second test allows to validate models adopted to close mass and energy source terms Γ_k and E_k. An isolated droplet with a diameter $d = 900$ µm and temperature 300K is initialised in a hot gas with temperature 1500K. Note that droplet diameter is deduced from α_l using eq. (8). The result provided by the Eulerian model presented in this paper is compared with that provided by the Lagrangian model already available in the code IFP-C3D. As shown in figures 7 and 8, which represent respectively the decrease of the square normalised diameter and the increase of the droplet temperature, the Eulerian model predicts a slightly smaller evaporation rate than the Lagrangian one. However, the droplet heating is very similar in the two computations. According to the fact that Eulerian simulation is not especially devoted to isolated droplet simulation, this result concerning evaporation is very satisfying. Indeed, Eulerian model is able to correctly reproduce isolated droplet evaporation, which is the worst test case that one can imagine.
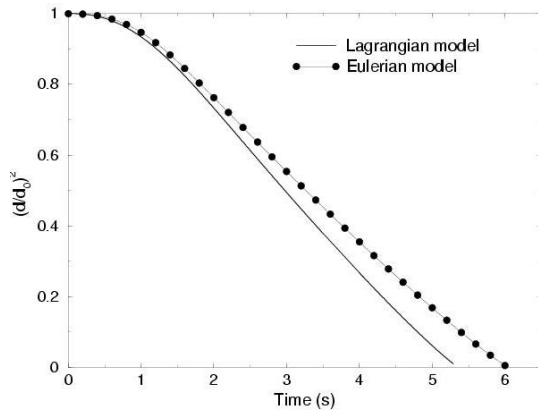

Figure 7: Evolution of the square normalised diameter for the evaporating droplet.
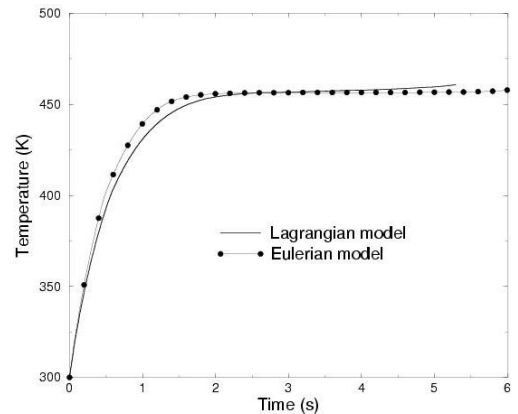

Figure 8: Evolution of the isolated droplet temperature.

4 - TOWARDS ENGINE COMPUTATIONS

In order to test the feasability of engine applications using the two-fluid-two-pressure model presented previously, a 2D simple test case has been achieved. In this test a liquid fuel (n-heptane) is injected with a velocity of 10 m/s and a temperature of 300K. The value of the liquid mass fraction at the injection boundary (of length 200µm, discretised with 10 cells) is chosen in such a way to have a droplet initial diameter of 20 µm. The initial temperature (resp. pressure) of the air contained in the computationnal domain (80*50 cells for 2mm*2.5mm) is 800K (resp. 10^5 Pa). Figure 9 shows the evolution of the liquid fuel volume fraction and the fuel vapour mass fraction along the time. One can notice in figure 10, which represents the evolution of the velocity field in the gaseous phase along the time, that liquid injection produces a pair of symetric vortices in the gas. On the other hand, lack of turbulence modelling leads to an undisturbed liquid spray. The behaviour and the robustness of our code are very encouraging for the next step that should be devoted to account for turbulent effects. At that moment, it will be possible to run a real engine case.
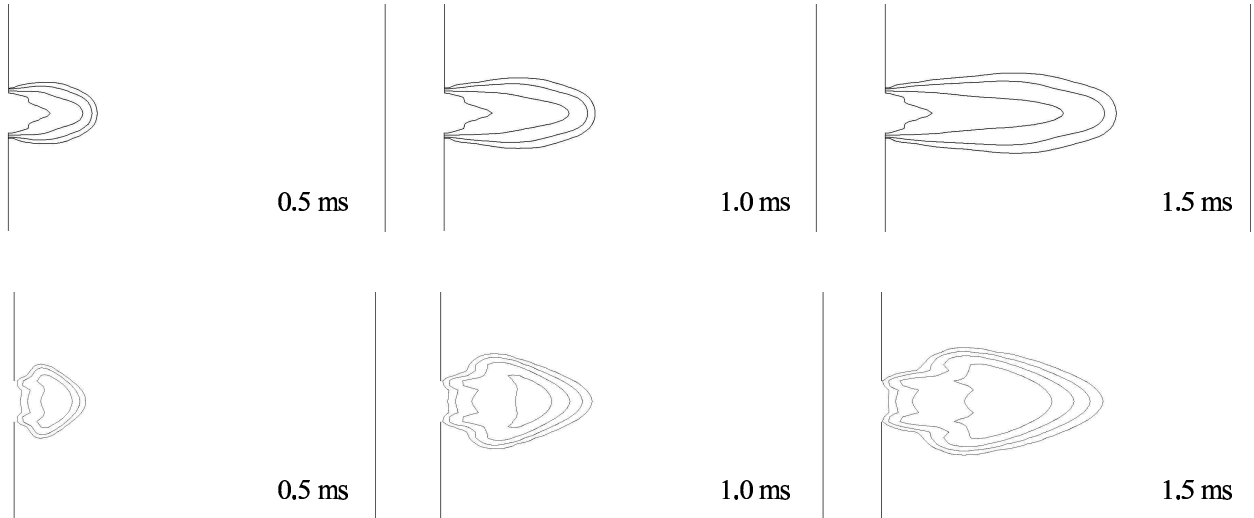

Figure 9 : Evolution of the liquid fuel volume fraction (isolines α_l = 0.05; 0.1; 0.2; 0.3 on the top line of figures) and the fuel vapour mass fraction (isolines 0.05; 0.1; 0.2; 0.4, on the bottom line of figures).
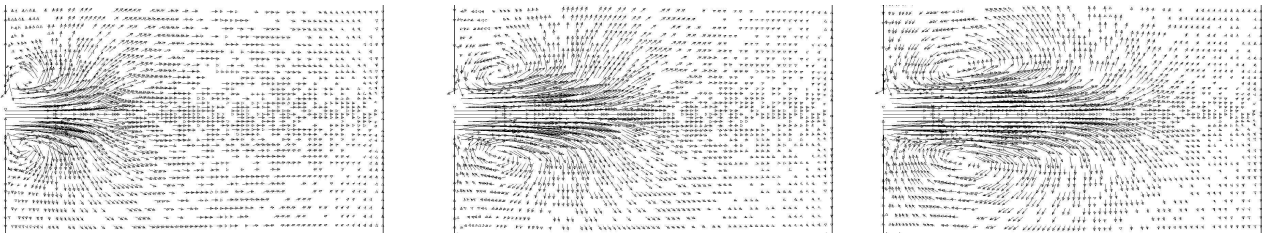

Figure 10 : Velocity field in the gas at t=0.5 ms,1 ms and 1.5 ms (from left to right).

5 - CONCLUSIONS AND FUTURE WORK

This paper has been devoted to the presentation of an Eulerian model developed to simulate two-phase flows in internal combustion engines. According to different physical constraints which appear in such an engine (especially the high injection velocity of the liquid fuel inside the combustion chamber), a two-fluid-two-pressure model has been chosen. The stiffened gas equation of state is used to compute the pressure in the liquid phase, whereas an ideal gas equation of state is used for the gaseous phase (fuel vapour and air). After a summarised description of the model, some indications, about approaches adopted to close source terms quantifying interfacial exchanges of mass momentum and energy between the liquid and the gaseous phases, are given. These closures are based on a spherical droplet assumption as a first approach that should be considered in future works. Several tests have been presented to validate the two-phase-two-pressure model implemented into the IFP code IFP-C3D. Some of these tests (the Poiseuille flow and the decay of the Green – Taylor vortex) aim at checking the correct implementation of the liquid phase transport equations. The other tests (the motion of droplets in a gas and the evaporation of an isolated droplet) allow to evaluate closures adopted for the interfacial source terms. Comparison with analytical solutions presented in this paper validate the basis

of the model. Finally a feasibility computation of a liquid fuel injection-evaporation into a 2D air vessel has been presented to show the robustness and the ability of the Eulerian model implemented into IFP-C3D. The current work is devoted to model turbulent effects that are not yet accounted for in the Eulerian model. This will allow to perform real engine applications in the near future.

ACKNOWLEDGMENTS

NOMENCLATURE

Latin symbols :
B_M : Spalding number (dimensionless)
C_V : heat capacity (J/kg/K)
d : caracteristic droplet diameter (m)
D : diffusion coefficient (m²/s)
e : internal sensible energy (J)
E : interfacial energy transfer (J.kg/m^3/s)
F_d : drag force (kg/m²/s²)
g : acceleration due to gravity (m/s²)
M : interfacial momentum transfer (kg/m²/s)
N : number of droplets (dimensionless)
Nu : Nusselt number (dimensionless)
P : pressure (Pa)

P_∞ : incompressibility coefficient (Pa)
Sh : Sherwood number (dimensionless)
t : time (s)
T : temperature (K)
U : velocity (m/s)
V : cell volume (m^3)
x,y,z : spatial direction (m)

Greek symbols :
α_κ : volume fraction of phase k (dimensionless)
γ : compressibility coefficient (dimensionless)
Γ : interfacial mass transfer (kg/m^3/s)

δ_I : Dirac distribution attached at the interface
λ : heat diffusivity coefficient (m²/s)
μ : dynamic viscosity (kg/m/s)
ρ : density (kg/m^3)
τ : viscous tensor (kg/m²/s)

Subscript :
g : gaseous phase
I : value attached with the interface
i,j : spatial direction
k : refered to one of the two phases
l : liquid phase

REFERENCES:

1. C. Hirt and B. Nichols, Volume of fluid (VOF) method for dynamics of free boundaries, *Journal of Computational Physics*, vol. 39, 1981.
2. Y. Chen, J. Glimm, D. Sharp and Q. Zhang, A two-phase flow model of the Rayleigh Taylor mixing zone, *Physics of fluids*, vol. 8 (3), pp.816-825, 1996.
3. A. Benkenida, Développement et validation d'une méthode de simulation d'écoulements diphasiques sans reconstruction d'interface, Application à la dynamique des bulles de Taylor, PhD thesis, INP Toulouse, 1999.
4. M. Ishii, Thermo-fluid theory of two phase flow, Eyrolles, 1975.
5. D. Drew, Mathematical modeling of two-phase flow, *Ann. Rev. Fluid Mech.*, vol 15, pp. 261-291, 1983.
6. R. Saurel and O. Lemetayer, A multiphase model for compressible flows with interfaces, shocks, detonation waves and cavitation, *Journal of Fluid Mechanic*, vol. 431, 2001.
7. E. Berg, A. Alajbegovic, R. Taschl, C. Krüger and U. Michels, Multiphase modeling of diesel sprays with the Eulerian/Eulerian approach, ILASS-Europe 2001.
8. O. Lemetayer, Modélisation et résolution de la propagation de fronts perméables application aux fronts d'évaporation et de détonation, PhD Thesis, Université de Provence, 2003.
9. O. Simonin, Combustion and turbulence in two-phase flows, Lecture Series 1996-02, Von Karman Institute for Fluid Dynamics, 1996.
10. V. Iyer, Modeling of diesel sprays using an Eulerian-liquid Eulerian-gas two fluid model, PhD Thesis, Faculty of Purdue University, 2001.
11. R. Menikoff and B. Plohr, The Riemann problem for fluid flow of real materials, *Reviews of modern physics*, vol.61 (1) pp. 75-130, 1989.
12. Kaufmann, Towards Eulerian-Eulerian large eddy simulation of reactive two phase flow, PhD Thesis, INP Toulouse, 2004.
13. H. Rusche, Computational fluid dynamics of dispersed two-phase flows at high phase fractions, PhD Thesis, Imperial College, 2002.
14. M. Zolver, D. Klahr, J. Bohbot, O. Laget and A. Torres, Reactive cfd in engines with a new unstructured parallel solver, *Oil & gas science and technology – Rev IFP*, 58 (1), pp 33-46, 2003.
15. I. Calmet, Analyse par simulation des grandes échelles des mouvements turbulents et du transfert de masse sous une interface plane, PhD thesis, INP Toulouse, 1995.