On the Polydisperse spray flames in turbulent flows using the 3D Euler-Euler approach

<u>L. Fréret</u>[★], O. Thomine[♦], J. Réveillon[♦]

S. de Chaisemartin^{\natural}, F. Laurent^{\sharp}, M. Massot^{\sharp}

★ Laboratoire LIP - UMR 7623
 ◊ Laboratoire CORIA, UMR 6614
 ‡ Institut Français du pétrole
 ‡ Laboratoire EM2C - Ecole Centrale Paris, UPR 288









Introduction

Numerical methods

Numerical simulations

3D Non-evaporating spray dispersion in a HIT gas flow Flame propagation from a hot spot in a monodispersed spray Flame propagation from a hot spot in a polydispersed spray 2D

Conclusions & Perspectives









New combustion chamber concepts \Rightarrow unsteadyness

Dispersed liquid phase + Large size spectrum

- Mixing of fuel vapor mass fraction and gazeous air
- stabilization
- combustion regimes











Modeling of the polydisperse spray

- ▶ Droplet / gas interactions
 ⇒ evaporation, drag and heat transfer
- ▶ Droplet / droplet interactions ⇒ Coalescence, break-up

Key parameter : size











Modeling of the polydisperse spray

- ▶ Droplet / gas interactions ⇒ evaporation, drag and heat transfer
- ► Droplet / droplet interactions ⇒ Coalescence, break-up

 $f^{\Phi}(t, x, \Phi, u_l, T_l)$: droplet density number (NDF)





Modeling of the polydisperse spray

- ▶ Droplet / gas interactions
 ⇒ evaporation, drag and heat transfer
- ► Droplet / droplet interactions ⇒ Coalescence, break-up

 $f^{\Phi}(t, x, \Phi, u_l, T_l)$: droplet density number (NDF)





Modeling of the polydisperse spray











Advantages & drawbacks

Lagrangian model :

- Modelisation
- Implementation
- gas-liquid coupling
- MPI parallelization

Eulerian model :

- Modelisation
- Implementation
- gas-liquid coupling
- MPI parallelization









Eulerian multi-fluid model

Conservation equations for each size interval :

$$\partial_t m^{(j)} + \partial_x (m^{(j)} u^{(j)}_d) = -(E_1^{(j)} + E_2^{(j)}) m^{(j)} + E_1^{(j+1)} m^{(j+1)}$$

$$\partial_t (m^{(j)} u^{(j)}_d) + \partial_x (m^{(j)} u^{(j)}_d \times u^{(j)}_d) = -(E_1^{(j)} + E_2^{(j)}) m^{(j)} u^{(j)}_d$$

$$+ E_1^{(j+1)} m^{(j+1)} u^{(j+1)}_d + m^{(j)} F^{(j)}$$





Eulerian multi-fluid model

Conservation equations for each size interval :

$$\partial_t m^{(j)} + \partial_x . (m^{(j)} u_d^{(j)}) = -(E_1^{(j)} + E_2^{(j)}) m^{(j)} + E_1^{(j+1)} m^{(j+1)} \\ \partial_t (m^{(j)} u_d^{(j)}) + \partial_x . (m^{(j)} u_d^{(j)} \times u_d^{(j)}) = -(E_1^{(j)} + E_2^{(j)}) m^{(j)} u_d^{(j)} \\ + E_1^{(j+1)} m^{(j+1)} u_d^{(j+1)} + m^{(j)} F^{(j)}$$

- Discretization of the size phase space is first order of accurate (Laurent 2001) number of sections (j) = number of equation systems number of sections increases dimension problem
- Recent developments of high order size moments (*PhD Thesis of D. Kah., 2010*)



Eulerian multi-fluid model

Conservation equations for each size interval :

$$\partial_t m^{(j)} + \partial_x (m^{(j)} u_d^{(j)}) = -(E_1^{(j)} + E_2^{(j)}) m^{(j)} + E_1^{(j+1)} m^{(j+1)} \\ \partial_t (m^{(j)} u_d^{(j)}) + \partial_x (m^{(j)} u_d^{(j)} \times u_d^{(j)}) = -(E_1^{(j)} + E_2^{(j)}) m^{(j)} u_d^{(j)} \\ + E_1^{(j+1)} m^{(j+1)} u_d^{(j+1)} + m^{(j)} F^{(j)}$$

- Discretization of the size phase space is first order of accurate (Laurent 2001) number of sections (j) = number of equation systems number of sections increases dimension problem
- Recent developments of high order size moments (*PhD Thesis of D. Kah*, 2010)
- mono-kinetic assumption at a given size, location and time Equivalent to pressureless gas dynamics

multi-fluid model

multi-velocity model







Introduction

Numerical methods

Numerical simulations

Conclusions & Perspectives









I) Splitting operator

Conservation equations for each size interval :

$$\begin{array}{lll} \partial_t m^{(j)} + \partial_x.(m^{(j)}u^{(j)}_d) &=& -(E^{(j)}_1 + E^{(j)}_2)m^{(j)} + E^{(j+1)}_1 m^{(j+1)} \\ \partial_t(m^{(j)}u^{(j)}_d) + \partial_x.(m^{(j)}u^{(j)}_d \times u^{(j)}_d) &=& -(E^{(j)}_1 + E^{(j)}_2)m^{(j)}u^{(j)}_d \\ && + E^{(j+1)}_1 m^{(j+1)}u^{(j+1)}_d + m^{(j)}F^{(j)} \end{array}$$



I) Splitting operator

Conservation equations for each size interval :

$$\partial_t m^{(j)} + \frac{\partial_{x.}(m^{(j)}u_d^{(j)})}{\partial_d} = -(E_1^{(j)} + E_2^{(j)})m^{(j)} + E_1^{(j+1)}m^{(j+1)}$$

$$\partial_t (m^{(j)}u_d^{(j)}) + \frac{\partial_{x.}(m^{(j)}u_d^{(j)} \times u_d^{(j)})}{\partial_d} = -(E_1^{(j)} + E_2^{(j)})m^{(j)}u_d^{(j)}$$

$$+ E_1^{(j+1)}m^{(j+1)}u_d^{(j+1)} + m^{(j)}F^{(j)}$$

- Transport in phase space during $\Delta t/2$ (evaporation, drag)
 - ODE equation



I) Splitting operator

Conservation equations for each size interval :

- Transport in phase space during $\Delta t/2$ (evaporation, drag)
 - ODE equation
- $\blacktriangleright\,$ Transport in physical space during Δt
 - weakly hyperbolic equation



I) Splitting operator

Conservation equations for each size interval :

$$\partial_t m^{(j)} + \partial_{\overline{x} \cdot (m^{(j)} u_d^{(j)})} = -(E_1^{(j)} + E_2^{(j)}) m^{(j)} + E_1^{(j+1)} m^{(j+1)}$$

$$\partial_t (m^{(j)} u_d^{(j)}) + \partial_{\overline{x} \cdot (m^{(j)} u_d^{(j)} \times u_d^{(j)})} = -(E_1^{(j)} + E_2^{(j)}) m^{(j)} u_d^{(j)}$$

$$+ E_1^{(j+1)} m^{(j+1)} u_d^{(j+1)} + m^{(j)} F^{(j)}$$

- ▶ Transport in phase space during $\Delta t/2$ (evaporation, drag)
 - ODE equation
- \blacktriangleright Transport in physical space during Δt
 - weakly hyperbolic equation
- $\blacktriangleright\,$ Transport in phase space during $\Delta t/2$
 - ODE equation









I) Splitting operator

i

Conservation equations for each size interval :

$$\partial_t m^{(j)} + \frac{\partial_{x\cdot}(m^{(j)}u_d^{(j)})}{u_d^{(j)}} = -(E_1^{(j)} + E_2^{(j)})m^{(j)} + E_1^{(j+1)}m^{(j+1)}$$

$$\partial_t (m^{(j)}u_d^{(j)}) + \frac{\partial_{x\cdot}(m^{(j)}u_d^{(j)} \times u_d^{(j)})}{u_d^{(j)}} = -(E_1^{(j)} + E_2^{(j)})m^{(j)}u_d^{(j)}$$

$$+ E_1^{(j+1)}m^{(j+1)}u_d^{(j+1)} + m^{(j)}F^{(j)}$$

Strang splitting algorithm :

- Transport in phase space during $\Delta t/2$ (evaporation, drag)
 - ODE equation
- \blacktriangleright Transport in physical space during Δt
 - weakly hyperbolic equation
- $\blacktriangleright\,$ Transport in phase space during $\Delta t/2$
 - ODE equation

divide problems into small sub-problems

second order in time and space









II) ODE resolution

stiffness :

evaporation, heat : temperature gradient

• drag :
$$F = \frac{1}{St} (\mathbf{U}_g - \mathbf{u}_l)$$

RadauIIA method ${}_{(Hairer)}$ 5th order in time, implicit RK, adaptative time step



III) Transport scheme

Strang dimensional splitting :

 $\Delta t \text{ transport} \Longrightarrow \begin{cases} \text{transport in x-direction during } \Delta t/2 \\ \text{transport in y-direction during } \Delta t/2 \\ \text{transport in z-direction during } \Delta t \\ \text{transport in y-direction during } \Delta t/2 \\ \text{transport in x-direction during } \Delta t/2 \end{cases}$

Equations equivalent to pressureless gas systems
$$\Longrightarrow \begin{cases} \partial_t \rho + \partial_x(\rho v) = 0\\ \partial_t(\rho v) + \partial_x(\rho v^2) = 0 \end{cases}$$

- Burger equation on velocity :
 - delta-shocks creation, vacuum density formation
- ▶ finite volume kinetic scheme (Bouchut 2003)
 - able to deal with delta-shocks and vacuum density
 - properties conservation
 - positivity of density
 - maximum principle on velocity









III) Transport scheme Strang dimensional splitting :

transport scheme in 1D, CFL=1

very limited numerical diffusion

Equations equivalent to pressureless gas systems $\Longrightarrow \begin{cases} \partial_t \rho + \partial_x(\rho v) = 0\\ \partial_t(\rho v) + \partial_x(\rho v^2) = 0 \end{cases}$

- ▶ Burger equation on velocity :
 - delta-shocks creation, vacuum density formation
- ▶ finite volume kinetic scheme (Bouchut 2003)
 - able to deal with delta-shocks and vacuum density
 - properties conservation
 - positivity of density
 - maximum principle on velocity









Muses3D code

- ▶ MUlti-fluid Solver for Eulerian Spray (S. de Chaisemartin, L. Freret)
- http://www.projet-plume.org/relier/muses3d
- ▶ multi-dimensional : 1D, 2D, 2D-axi, 3D
- multi-solver
 - multi-fluid model
 - mutli-fluid multi-velocity model
 - multi-fluid multi-size model
- \blacktriangleright gas/droplet interactions
 - evaporation
 - drag
 - heat transfer
- ▶ droplet/droplet interactions
 - collisions









Introduction

Numerical methods

Numerical simulations

3D Non-evaporating spray dispersion in a HIT gas flow Flame propagation from a hot spot in a monodispersed spray Flame propagation from a hot spot in a polydispersed spray 2D

Conclusions & Perspectives









I) 3D Non-evaporating spray dispersion in a HIT gas flow

Goals

- ▶ Spray repartition study in a 3d instationnary context
- ▶ Comparisons between Eulerian and Lagrangian liquid phase
- ▶ Coupling multi-fluid with Euler-Lagrange code Asphodele (J. Réveillon, Coria)

(Fréret & al., ICMF 2010)

Gas phase

- Homogeneous isotropic turbulent instationnary flow
- ▶ Re=1000, turbulence forcing method
- ▶ Spatial discretization 129^3



vorticity field





I) 3D Non-evaporating spray dispersion in a HIT gas flow

Liquid phase

- ▶ Homogeneous repartition of the spray liquid phase
- ▶ Non-evaporating mono-dispersed droplets, Stokes=0.2
- ▶ only 1 section for MF model
- $\blacktriangleright~1$ droplet per mesh cell \simeq total particle number 2,150,100



I) 3D Non-evaporating spray dispersion in a HIT gas flow

Liquid phase

- ▶ Homogeneous repartition of the spray liquid phase
- ▶ Non-evaporating mono-dispersed droplets, Stokes=1
- ▶ only 1 section for MF model
- $\blacktriangleright~1$ droplet per mesh cell \simeq total particle number 2,150,100



I) 3D Non-evaporating spray dispersion in a HIT gas flow

Liquid phase

- ▶ Homogeneous repartition of the spray liquid phase
- ▶ Non-evaporating mono-dispersed droplets, Stokes=1
- ▶ only 1 section for MF model
- $\blacktriangleright~1$ droplet per mesh cell \simeq total particle number 2,150,100











I) 3D Non-evaporating spray dispersion in a HIT gas flow

Scientific computing

- Entire gas velocity field known on each core
- \blacktriangleright No evaporation / no collision \Longrightarrow droplets are independent
- Equivalent to Monte Carlo simulations
 - no communication between cores
 - optimal parallelization for the Lagrangian liquid phase
- ▶ 32 cores \implies total particule number / 32 = 65,000 per core



II) Flame propagation from a hot spot in a monodispersed spray 2D

Goals

- ▶ Capacity of the multi-fluid method to simulate combustion process
- ▶ Influence of segregation onto evaporation and combustion process
- ▶ Cool flame configuration (no heat transfer)
- ▶ Comparisons between Eulerian and Lagrangian liquid phase

(Fréret & al., CTR 2010)

Gas phase

- Homogeneous isotropic turbulent instationnary flow
- ▶ Re=1000, turbulence forcing method
- ▶ Spatial discretization 256²
- ▶ Hot spot in the domain center



vorticity field







II) Flame propagation from a hot spot in a monodispersed spray 2D

Liquid phase

- ▶ Heterogeneous repartition of the spray liquid phase
- ▶ Evaporating initially mono-dispersed droplets, Stokes=0.2
- ▶ 20 sections for MF model (discretization : 512^2)
- $\blacktriangleright~1$ droplet per mesh cell \simeq total particle number 70,000

Eul. density

Lag. density





II) Flame propagation from a hot spot in a monodispersed spray 2D

Liquid phase

- ▶ Heterogeneous repartition of the spray liquid phase
- ▶ Evaporating initially mono-dispersed droplets, Stokes=0.2
- ▶ 20 sections for MF model (discretization : 512^2)
- $\blacktriangleright~1$ droplet per mesh cell \simeq total particle number 70,000

Evolution of Eulerian mass density repartition







II) Flame propagation from a hot spot in a monodispersed spray 2D

Fuel mass fraction comparison (top : Eulerian, bottom : Lagrangian)



Time







II) Flame propagation from a hot spot in a monodispersed spray 2D

Front flame propagation (top : Eulerian, bottom : Lagrangian)



Time





II) Flame propagation from a hot spot in a monodispersed spray 2D

Front flame propagation (top : Eulerian, bottom : Lagrangian)



Time







II) Flame propagation from a hot spot in a monodispersed spray 3D

Fuel mass fraction comparison (top : Eulerian, bottom : Lagrangian)





Time







II) Flame propagation from a hot spot in a monodispersed spray 3D

Front flame propagation (top : Eulerian, bottom : Lagrangian)





Time







II) Flame propagation from a hot spot in a monodispersed spray 3D

Scientific computing

- Evaporation process \implies exchange between gas and liquid phase
- Classical spatial domain decomposition
 - a lot of communication between cores for the Lagrangian liquid phase
- ▶ 512 cores \implies total particule number / 512 \simeq 5,000 per core





III) Flame propagation from a hot spot in a polydispersed spray 2D

Liquid phase

- ▶ Heterogeneous repartition of the spray liquid phase
- \blacktriangleright Evaporating initially poly-dispersed droplets, Stokes = 0 $\longrightarrow 1.32$
- ▶ 20 sections for MF model / 100 droplets per mesh cell \simeq total > 6,500,000



III) Flame propagation from a hot spot in a polydispersed spray 2D

Fuel mass fraction comparison (top : Eulerian, bottom : Lagrangian)









III) Flame propagation from a hot spot in a polydispersed spray 2D

Front flame propagation (top : Eulerian, bottom : Lagrangian)



Time





III) Flame propagation from a hot spot in a polydispersed spray 2D

Front flame propagation (top : Eulerian, bottom : Lagrangian)



Time







Introduction

Numerical methods

Numerical simulations

Conclusions & Perspectives









Conclusions

- ▶ Capacity of the multi-fluid method to deal with 3d configurations
- ▶ Comparison of combustion process between Lagrangian & Eulerian description
- ▶ Qualitative & quantitative comparisons between Eul. and Lag. model
- ▶ Use of numerical method adapted to parallel computing
- Splitting algorithm
 - Transport in phase space / Transport in physical space
 - Dimensional splitting
- Very good scaling









Perspectives

- $\blacktriangleright\,$ 3D combustion process with a polydispersed evaporating spray
- ▶ Take into account heat tranfer
- ▶ Comparison of auto-ignition delay (PhD. of Zakaria Bouali)

First results

- Homogeneous spray liquid repartition
- Quiescent atmosphere
- Complex kinetic
- Heat transfer
- Initial temperature gas : 750K, 900K et 1200K







References

L. Freret, O. Thomine, J. Reveillon, S. de Chaisemartin, F. Laurent, M. Massot On the role of preferential segregation in flame dynamics in polydisperse evaporating sprays Proceedings of the summer Program 2010, Center for turbulence research

L. Freret, S. de Chaisemartin, J. Reveillon, F. Laurent, M. Massot Eulerian models and three-dimensional numerical simulation of polydisperse sprays 7th international conference on multiphase flows. ICMF 2010

S. de Chaisemartin, L. Freret, D. Kah, F. Laurent, R.O.Fox, J. Reveillon, M. Massot Turbulence combustion of polydisperse evaporating sprays with droplet crossings : Eulerian modeling and validation in the infinite Knudsen limit Proceedings of the summer program 2008, Center for Turbulence Research

S. de Chaisemartin, PhD Thesis, 2009 Modeles euleriens et simulation numerique de la dispersion turbulente de brouillards qui s'evaporent, http://tel.archives-ouvertes.fr/tel-004/43982/fr/

D. Kah, PhD Thesis, 2010

J. Reveillon, F.X. Demoulin Effects of the preferential segregation of droplets on evaporation and turbulent mixing J. Fluid Mech, 2007

M. Massot, S. de Chaisemartin, L. Freret, D. Kah, F. Laurent Eulerian multi-fluid models : modeling and numerical methods in modelling and computation of nanoparticles in fluid flows, Lectures of the von Karman Institute 2009

M. Massot Eulerian multi-fluid modelling for polydisperse evaporating sprays Chap. III of Multiphase reacting flows : modelling and simulation, Series : CISM International Centre for Mechanical Sciences (2007)

D. Kah, F. Laurent, L. Freret, S. de Chaisemartin, R. O. Fox, J. Reveillon, M. Massot Eulerian quadrature-based moment models for dilute polydisperse evaporating sprays, Flow Turbulence and Combustion, 2010







