Some aspects of turbulent mixing in two phase flows

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Matsui-Kosaka



Key phenomena is "turbulent" mixing



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Out line

Part I : Introduction to atomization and two-phase flow modeling Part II : Turbulence mixing approach for atomization



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Fundamentals:

Experimental observations





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C. Dumouchel, Heat and mass transfer in spray systems, 2005



Influence of inlet velocity profile

- •d = 2.54 mm•Glycerol-eau/air • $U_L = 20 \text{ m/s}$ • $We_G = 15$
- •Photos : Mc Carthy et Molloy, 1973



•The relaxation of the velocity profile may generate instabilities that promote the atomization process



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REACCHINE

C. Dumouchel, Heat and mass transfer in spray systems, 2005

Influence liquid viscosity



Air assisted Atomization

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Air assisted atomization (Co-axial jets)





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Basic phenomena:

Linear instabilities



Kelvin – Helmholtz instability





Kelvin – Helmholtz instability

Main results:



Dispersion diagram: Kelvin – Helmholtz instability





Rayleigh-Taylor instability







Rayleigh-Plateau instability











\rightarrow To understand physical phenomena

\rightarrow To give an explanation of droplet formation



P. H. Marmottant and E. Villermaux, Journal of Fluid Mechanics 498 (498), 73 (2004)





Two-phase flows:

Main formalisms



Generally based on dispersed phase (at less discrete)

 \rightarrow A carrier phase can be defined, ex: GAS

→ Transported discrete particles, ex: DROPLET

→ Few parameters are involved:

u(t), droplet velocity X(t), droplet centre position D: diameter

But also:

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Droplet temperature, concentration, departure to sphericity, ...

Gas characteristics seen by droplet: velocity, temperature, concentration,...



Statistical description:

Joint distribution of drop characteristic $\rightarrow f(X_E, t, D, u, T, ...)$

Boltzmann-Williams equation:

$$\begin{aligned} \frac{\partial f}{\partial t} + \frac{\partial \dot{x}_i f}{\partial x_i} + \frac{\partial \dot{u}_i f}{\partial u_i} + \frac{\partial \dot{D} f}{\partial r} + \frac{\partial \dot{T} f}{\partial T} &= \Gamma \\ \frac{\partial \dot{A} f(x_i, t, u_i, D, T)}{\partial A} \Rightarrow \dot{A} &= \left\langle \dot{A}(x_i, t, u_i, D, T, u_{i,g}, T_g, ... \right\rangle \Big|_{x_i, t, u_i, D, T} \end{aligned}$$

Position: $\dot{x}_i = u_i$ Evaporation (D² law) :

$$\dot{D} = \left\langle \dot{D}(x_i, t, u_i, D, T, u_{i,g}, T_g, \dots) \right|_{x_i, t, u_i, D, T}$$
$$\dot{D} = \left\langle \frac{\rho_g}{\rho_l r} D_v Sh(\operatorname{Re}_d = \frac{2r \left\| \vec{u} - \vec{u}_g \right\|}{V_g}, S_c) \ln \left(\frac{1 - Y_v}{1 - Y_{vs}} \right) \right\rangle \right|_{x_i, t, u_i, r, T}$$



Many methods: focus on the diameter distribution



Lagrangian Models: Direct resolution of the B.-Williams equation

Monte-Carlo approach: a set of sample (droplet) is followed

For each droplet, characteristic evolution is solved (Lagrangian)

$$\begin{cases} \frac{dx_i}{dt} = \dot{x}_i = u_i \\ \dot{u}_i = drag + gravity + \dots \\ \dot{D} = breakup + evaporation + \dots \\ \dot{T} = heat transfer \end{cases}$$

Statistic are obtained by summing over droplet samples

« Lagrangian Method »,« DDM Dispersed Droplet Model »

Dukowicz₁₉₈₀



Application to atomization → Lagrangian Methods



Lagrangian Models: Primary Atomization

Reitz model (*A&S 1987*) or « Wave model » : *Surface instability :Kelvin –Helmholtz*





Kelvin-Helmholtz, Wave model (R. Reitz, A&S 1987)

Spay angle:
$$tg\left(\frac{\theta}{2}\right) = A_1 \Lambda \Omega u_0$$

Bulk velocity: $u_0 = c(2\Delta p / \rho_1)$, c :discharge coefficient

Break-up: parent drop radius a and child drop radius r

$$\frac{da}{dt} = -\frac{(a-r)}{\tau}$$
 with $\tau = 3.726 B_1 \frac{a}{\Lambda\Omega}$

$$r = \begin{cases} B_0 \Lambda & \text{if } B_0 \Lambda \le a \\ \min\left[\left(\frac{3\pi a^2 u_l}{2\Omega}\right)^{\frac{1}{3}}; \left(\frac{3a^2 \Lambda}{4}\right)^{\frac{1}{3}}\right] & \text{if } B_0 \Lambda > a, \text{ only one time} \end{cases}$$



Results/ Experiment



It works ..., but "constants" are dependent of the injector. How to take into account complicated injector geometry ?



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Part III : Turbulence, droplet, vaporization, mixing and combustion



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ELSA model

Eulerian Lagrangian Spray Atomisation



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ElSA model in action:



Dense Eulerian Model

Diluted Lagrangian Model



Application to air-blast atomization


Eulerian description of primary break-up mixture flow

A single flow with two species: Gas Y_{s} and Liquid Y_{i} Mean velocity, pressure and density : \tilde{U}_{i} , \bar{p} , $\bar{\rho}$ Turbulence: $k - \varepsilon$ model or second order models

Transport of the liquid species:

 $\frac{\partial \overline{\rho} \widetilde{Y}_{i}}{\partial t} + \frac{\partial \overline{\rho} \widetilde{U}_{j} \widetilde{Y}_{i}}{\partial x_{j}} = -\frac{\partial \overline{\rho} u_{j}^{"} Y_{i}^{"}}{\partial x_{j}}$

Turbulent liquid mass flux $\frac{\partial}{\partial x_{i}} \overline{\rho} \frac{V_{i}}{D_{i}} \frac{\partial \widetilde{Y}_{i}}{\partial x_{i}} \qquad ??$

Mean velocity \leftarrow NOT \rightarrow Equal velocity: $\left|\overline{U_i}\right|_g \neq \overline{U_i}$

$$\overline{\rho u_i^{"} Y_i^{"}} = \overline{\rho} \widetilde{Y}_i \widetilde{Y}_g (\overline{U}_i \big|_l - \overline{U}_i \big|_g) = \overline{\rho} \widetilde{Y}_l (\overline{U}_i \big|_l - \widetilde{U}_i)$$



Modelling turbulence for flows with high density fluctuations



Test first and second order model ...



Figure 2: Profiles of the liquid volume fraction along the main axis. The curve with symbols corresponds to experimental data [21]. The regular curves are the result of calculation with:

$$1 = k - \varepsilon; \qquad 2 = k - \varepsilon + G_k; \qquad 3 = k - \varepsilon, D_t \times 10; \qquad 4 = k - \varepsilon + G_k, D_t \times 10; \qquad 5 = R_{ij} - \varepsilon, R_{iY_i} = K - \varepsilon + G_k, D_t \times 10; \qquad 5 = R_{ij} - \varepsilon, R_{iY_i} = K - \varepsilon + G_k, D_t \times 10; \qquad 5 = K - \varepsilon + G_k = K -$$

 $6 = R_{ij} - \varepsilon + G_{ij}, R_{iY_l} + G_{I_i}; 7 = R_{ij} - \varepsilon + G_{ij}, D_t$

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F.-X. Demoulin et al, Atomization and Sprays, 2007

Turbulent modeling of the $\rho u''_{i} Y''$ equation





Rayleigh Taylor Instability





Turbulent Jet



Hopfinger et al

Not so clear !

Ligaments: Yes

Increase of $\overline{\rho u_i^{"}Y_i}$: Probable



New modeling of the $\rho u''_{i} Y''$ equation

Increase of turbulent dispersion due to gravity effect Lumley (1975) and Launder (1975)

$$p'\frac{\partial Y_l''}{\partial x_i} = \dots + C_{y3}\overline{\rho}(1/\rho_l - 1/\rho_g)\overline{\rho}Y_l''Y_l''g_i$$

New model: replacing gravity by a turbulent acceleration

$$\overline{p'\frac{\partial Y_{i}''}{\partial x_{i}}} = \dots + C_{yr}\left(\frac{1}{\rho_{i}} - \frac{1}{\rho_{g}}\right)\overline{\rho Y_{i}''Y_{i}''}\overline{\rho v''v''}\frac{\partial \widetilde{Y_{i}}}{\partial x_{i}}$$

$$-\overline{\rho v''Y''} \approx \left(\overline{\rho v''v''} \frac{k}{a_1 \varepsilon} + \frac{C_{yr}}{a_1} \frac{k}{\varepsilon} \overline{\rho v''v''} \widetilde{Y}(1-\widetilde{Y})(\frac{\overline{\rho}}{\rho_g} - \frac{\overline{\rho}}{\rho_l})\right) \frac{\partial \widetilde{Y}}{\partial y}$$



Model effect of variable density

Standard model:

$$\overline{\rho u''_{i} Y''_{i}} = -\overline{\rho} \frac{V_{t}}{Sc_{t}} \frac{\partial \widetilde{Y}_{i}}{\partial x_{i}}$$
New model: $\overline{\rho u''_{i} Y''_{i}}$

$$= -\overline{\rho} \left(\frac{V_{t}}{Sc_{t}} + C_{\rho} \frac{k^{2}}{\varepsilon} \overline{\rho} (1/\rho_{s} - 1/\rho_{t}) \widetilde{Y}_{i} (1 - \widetilde{Y}_{t}) \right) \frac{\partial \widetilde{Y}_{t}}{\partial x_{i}}$$

$$= -\overline{\rho} \left(\frac{V_{t}}{Sc_{t}} + C_{\rho} \frac{k^{2}}{\varepsilon} |\overline{Y}_{t}^{"}| \right) \frac{\partial \widetilde{Y}_{t}}{\partial x_{i}}$$
Where $V_{t} = c_{\mu} \frac{k^{2}}{\varepsilon}, c_{\mu} = 0.09, Sc_{t} = 0.9$ and $C_{\rho} = 1.8$







F.-X. Demoulin et al, Atomization and Sprays, 2007



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J=5.88





J=3.04





J=1.47







Application of ELSA model to Diesel atomization



Direct numerical simulation ...

T. Ménard, S. Tanguy, A. Berlemont



Push at its limit

Physical case

Characteristics of the spray :

Diameter (D)	velocity	Turbulent intensity	Lenght scale
100 μm	100 m.s ⁻¹	u'/U=0.05	0.1D
phase	Density	Viscosity	Surface tension
Liquid	696 kg.m ⁻³	1.2 10 ⁻³ kg.m ⁻¹ .s ⁻	0.06 N.m ⁻¹
gas	25 kg.m ⁻³	1. 10 ⁻⁵ kg.m ⁻¹ .s ⁻¹	

Instantaneous Turbulent inflow : (Klein 2003)





Simulation of primary breakup (Diesel conditions)



Coupling level set/VOF/ghost fluid methods: Validation and application to 3D simulation of the primary break-up of a liquid jet T. Menard, S. Tanguy, A. Berlemont, IJMF 2007



Morphology





Model Comparisons

P.A. Beau, R. Lebas



Liquid volume fraction comparison

Transport of the liquid species:

$$\frac{\partial \overline{\rho} \widetilde{Y}_{l}}{\partial t} + \frac{\partial \overline{\rho} \widetilde{U}_{j} \widetilde{Y}_{l}}{\partial x_{j}} = \frac{\partial}{\partial x_{j}} \left(\overline{\rho} D_{t} \frac{\partial \widetilde{Y}_{l}}{\partial x_{j}} \right)$$
$$D_{t} = C_{\mu} \frac{k^{2}}{\varepsilon}$$

Classical turbulent diffusion + k- ϵ



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Axial profile





Radial profiles





Surface density comparison

$$\frac{\partial \overline{\Sigma}}{\partial t} + \frac{\partial \widetilde{u}_j \overline{\Sigma}}{\partial x_j} = \frac{\partial}{\partial x_j} \left(D_t \frac{\partial \overline{\Sigma}}{\partial x_j} \right) + \left(\left| A \right| + a_{coll} \right) \cdot \overline{\Sigma} - V_s \cdot \overline{\Sigma}^2$$

•Production due to the mean flow stretching

$$A = \alpha_0 \frac{\rho u''_i u''_j}{\overline{\rho}k} \frac{\partial \widetilde{u}_i}{\partial x_j}$$

•Production due to collision effects

$$a_{coll} = \frac{\alpha_1}{(36\pi)^{2/9}} \left(l_t \overline{\Sigma} \right)^{2/3} \left(\frac{\rho_l}{\overline{\rho} \widetilde{Y}_l} \right)^{4/9} \frac{\varepsilon}{k}$$

•Equilibrium, surface tension effect

$$V_s = \frac{a_{coll}\rho_l r_{eq}}{3\overline{\rho}\widetilde{Y}_l} \qquad r_{eq} = C \frac{\sigma^{3/5} l_t^{2/5}}{k} \frac{\left(\overline{\rho}\widetilde{Y}_l\right)^{2/15}}{\rho_l^{11/15}}$$

COMPLEXE DE RECHERCHE INTERPROFESSIONNEL EN ABROTHERMOCHIMIE

A. Vallet, A. A. Burluka and R. Borghi, Atomization and Sprays, 2001

Axial profile





Radial profiles



Distance from the axis (Y/D)



Conclusions and perspectives

→Global turbulent approach (like k- ε) can be applied to describe first atomization for high Weber and Reynolds number

 \Rightarrow Such models are necessarily to couple atomization with injector flow

→ Liquid dispersion in such cases can be described like turbulent mixing accurately

→Main instability mechanisms should be incorporated in the model

→ Still very complex phenomena are involved in addition to 'regular' turbulence

→ How things would be improved by using LES ?



GOAL : LES of atomisation

Test coaxial injector:





Contours of Volume fraction (phase-1) (Time=4.6034e-D3)

Mar D9, 2007 FLUENT 6.3 (3d, pbns, vof, LES, unsteady)







GOAL : LES for velocities and liquid/interface TO the SPRAY

Mean



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Once the droplet are formed ...



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Configuration: isotropic turbulence



Gas Phase: DNS

- Spectral resolution
- Semi-deterministic forcing scheme
- Statistically stationary properties (u', l_t, \mathcal{E})

Dispersed Phase: Lagrangian solver

- 1-way momentum, 2-way vapor
- Monodispersed spray
- Control parameter:

Stokes number: $St = \frac{\tau_p}{\tau_\eta}$



 129^3 nodes and $> 10^6$ droplets



2. Spray dynamical equilibrium

3. Liquid phase evaporation



A 4 step numerical procedure

1. Statistically stationary turbulence



4. Flame ignition and propagation



Liquid density: ξ , mean value: $\overline{\xi} = 1$







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Segregation efficiency:

Droplet ejection ⇔Turbulent mixing⇔Ballistic trajectories



Impact on Evaporation

Z= vapour mass fraction



•Case C (heavy) evolves from A to B: C \Leftrightarrow A \rightarrow C \Leftrightarrow B

Segregation \rightarrow up to 100% variation on *Z*'


Liquid segregation and Stokes number evolution



•Evaporation \rightarrow evolution of Stokes number

•Case C : first segregation increases

•Case C merges with case B when St = 1

CONFIENE DE RECHERCHE MILTERROSPERIONNEL EN ABROTHERMOCHIMIE

Evaporation regimes

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PDF shape and evolution





Energy Spectra of Z and ξ



St = 0.17



St = 5.06



Summary for segregation on evaporation:

	\overline{Z}	Ζ'	P(Z)	E_{Z}	E_{ξ}
$t \approx 0$	-			+	+
$0 < t < \tau_v$	+	++	++	+/	+
$t > T_{v}$		++		_	+



Globally premixed flame propagation:



Case B



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Mean Flame Radius vs Time:



Late ignition: $\tau_{ign} = \tau_v$ and $u_l < u'$

 \rightarrow weak influence of segregation on flame propagation

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Scatter plot: reaction rate vs mixture fraction



Same mean behaviour but different local flame structures



Conclusion for segregation effect on evaporation

- •Liquid density ξ characterises the spray segregation
- •Parallel comparisons of liquid and vapour fields
- •First two moment of ξ insufficient to characterise segregation

→ Topological information needed

- •The segregation plays a major role on vapour fluctuations
- •For $\tau_{ign} = \tau_v$ and $u_l < u'$ turbulence flame speed not really affected
- •Still, local flame structure is influenced



Conclusions & Perspectives

- Certain aspects of two-phase flow involved turbulence
- Additional phenomena have to be taken into account:
 - Inertia, surface tension, phase change ...
- → Still many open questions
- But in some cases, classical turbulence approaches give interesting results





... thank you for your attention.



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