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INSTITUT  
DE RADIOPROTECTION  
ET DE SÛRETÉ NUCLÉAIRE



Laboratoire d'Energétique et de  
Mécanique Théorique et Appliquée

# Secondary breakup in the context of Fuel Coolant Interactions (FCI)

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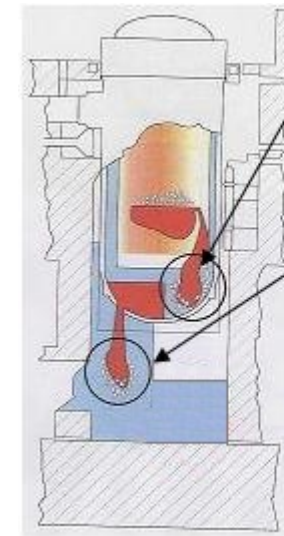
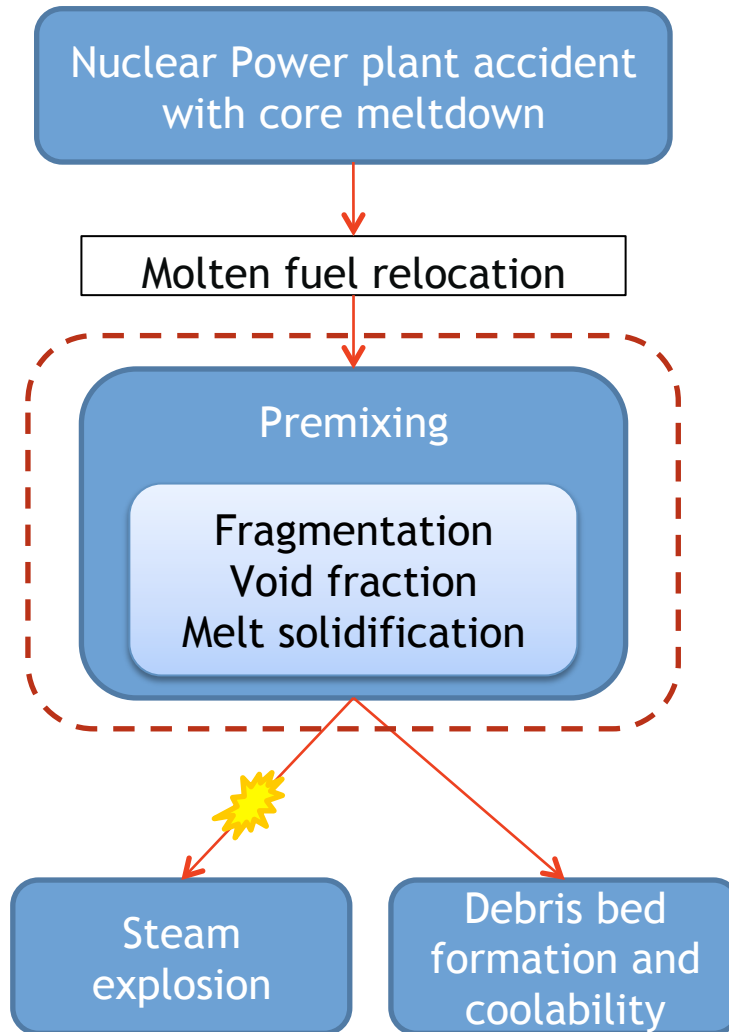
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# Planning

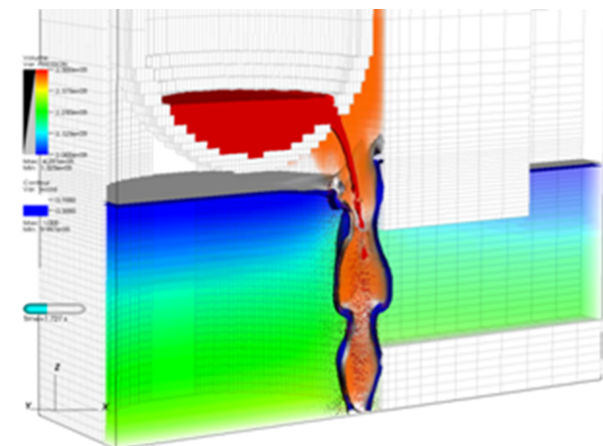
- General description of Fuel Coolant Interactions (FCI)
- Numerical resources at IRSN to evaluate FCI: MC3D
- Primary and secondary fragmentation
- Secondary fragmentation during FCI
- Drop breakup in liquid/gas and liquid/liquid environments
- Some results using MC3D
- Drop breakup using Gerris code
- Some results and ways of improvement

# Fuel Coolant Interactions (FCI)



In-vessel configuration

Ex-vessel configuration



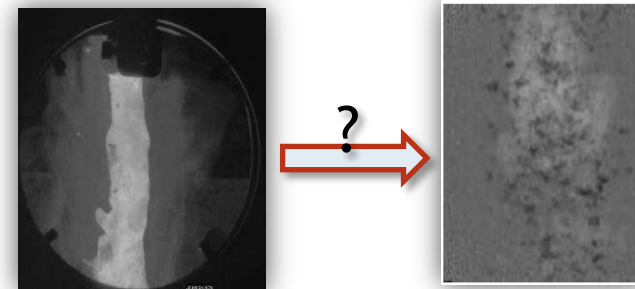
Example of a 3D calculation with MC3D

# Position of the problem of corium fragmentation

How a coherent melt jet is transformed into droplets or fragments ?

## Particular difficulties :

- Highly non-linear and unstable phenomenon with strong feedback
- Impact of melt solidification and oxidation with complex melt compositions
- physical properties quite uncertain



Krotos KS4

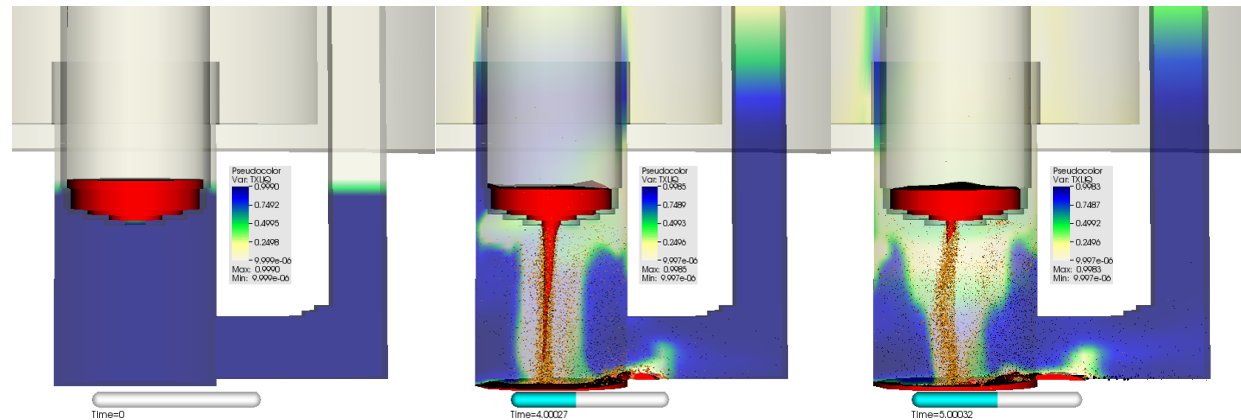
# FCI simulation at IRSN; CFD code MC3D

Multiphase code MC3D

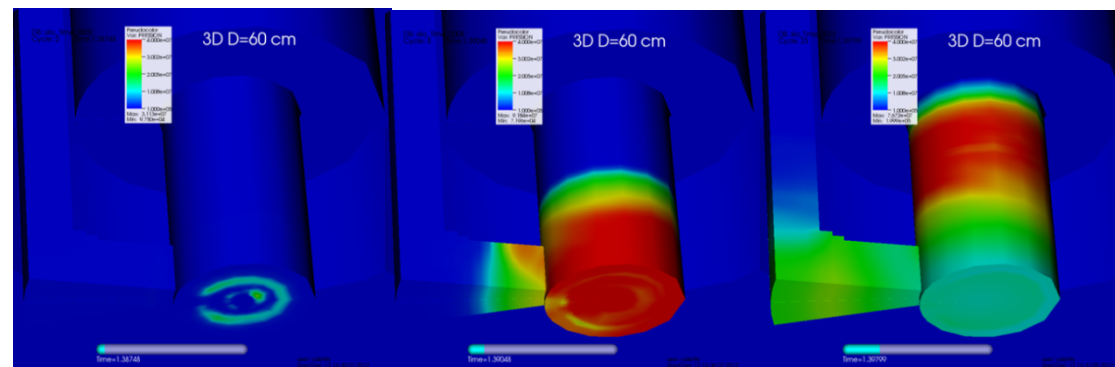
Different fluid fields:

- Liquid coolant and steam + non condensable gases (H<sub>2</sub>, O<sub>2</sub> ...)
- Jet (Unfragmented melt, with an interface tracking VOF-PLIC method)
- Dispersed melt droplets

PREMIXING



EXPLOSION



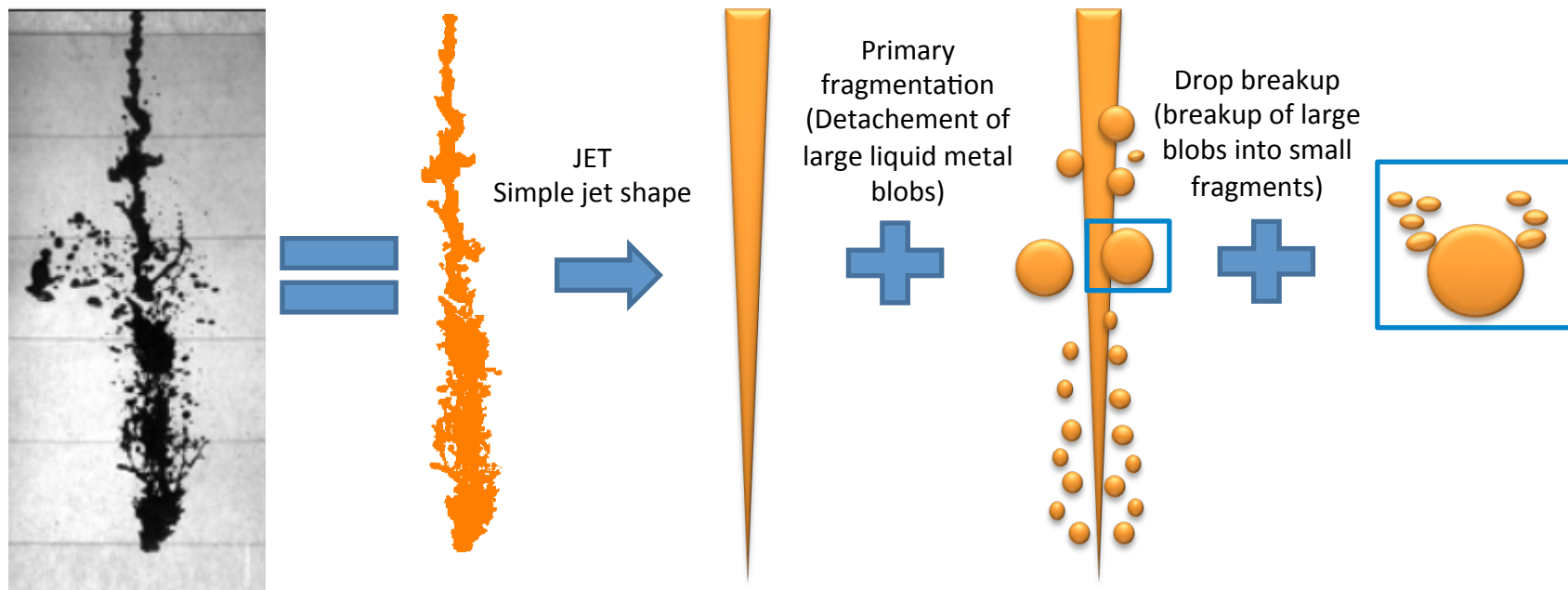
# Melt jet fragmentation during premixing

- Primary fragmentation

Large scale jet destabilisation - Detachment of large blobs from jet

- Secondary fragmentation

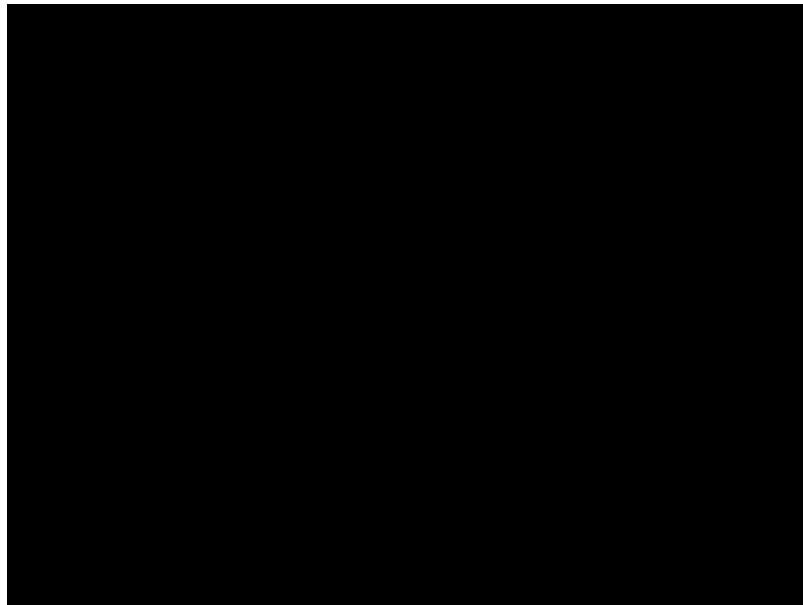
Breakup of blobs and droplets following local scale hydrodynamic conditions



Matsuo et al. 2008

# Secondary fragmentation on FCI

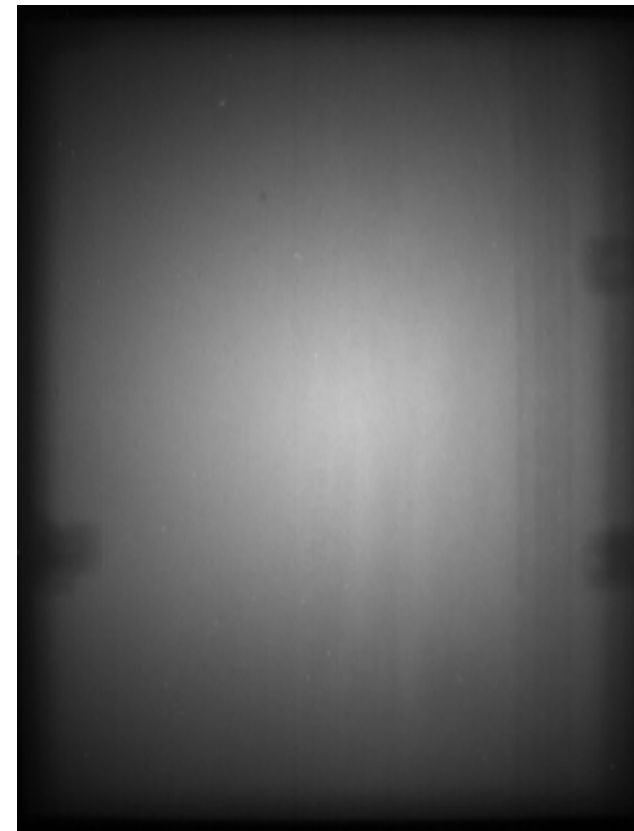
Jet injection and  
premixing zone



Secondary breakup during:

- Free fall of jet
- Contact of corium blobs with water flow
- High speed counter flow

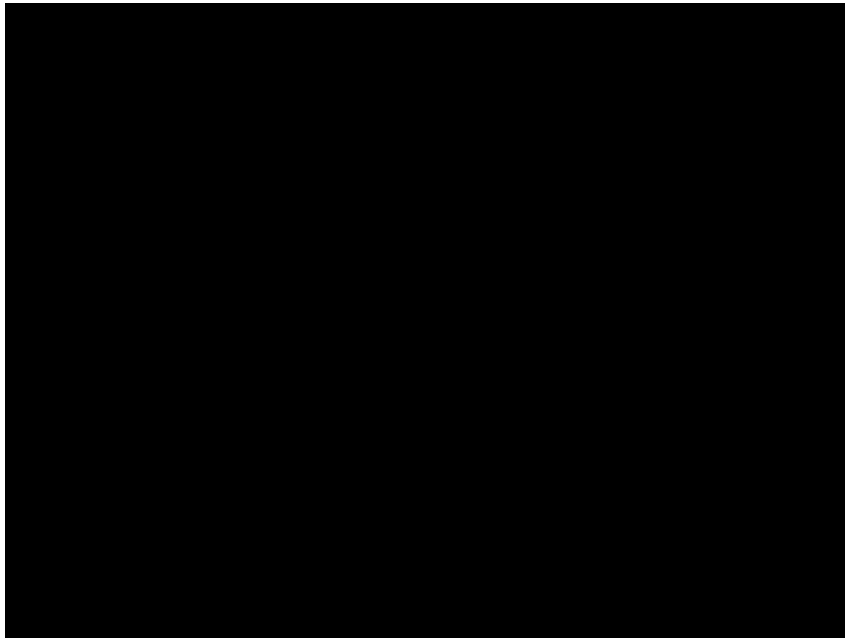
Watching the premixing  
zone with X-ray !!!



Krotos KS4

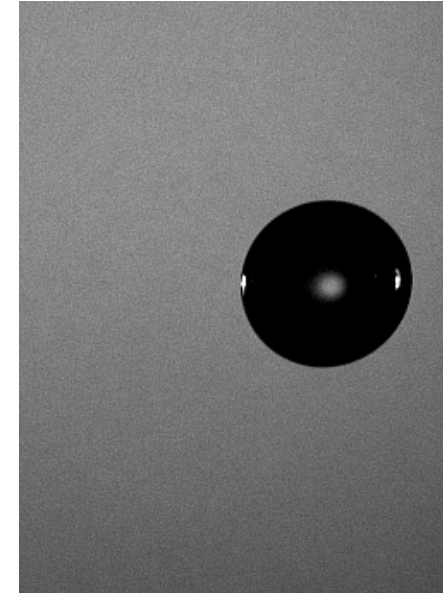
# Secondary fragmentation on FCI

Liquid Metal-liquid configuration  
1000°C Tin droplet in water



De Malmazet 2009

Liquid-gas configuration



Theofanous et al. 2012

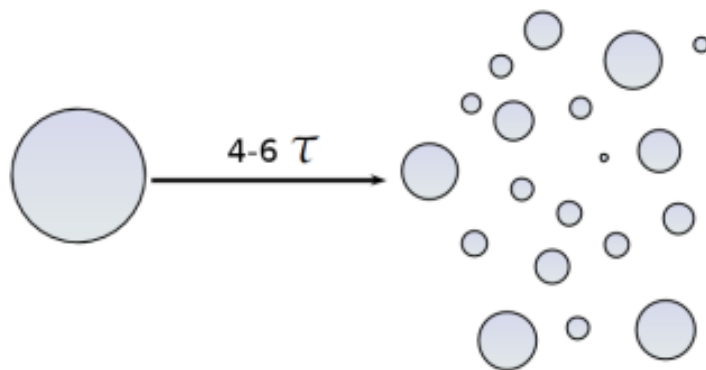
Preliminary hypothesis on secondary breakup during FCI:

- Hydrodynamic fragmentation controls the global behavior of breakup
- Weak influence of local thermal interactions
- Weak influence of steam film around droplets
- Breakup following pure liquid/gas or liquid/liquid configuration



# Modelling hypothesis

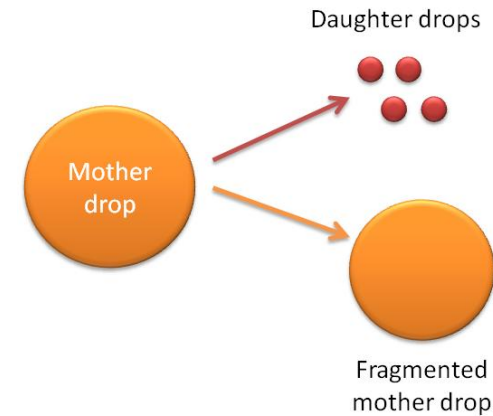
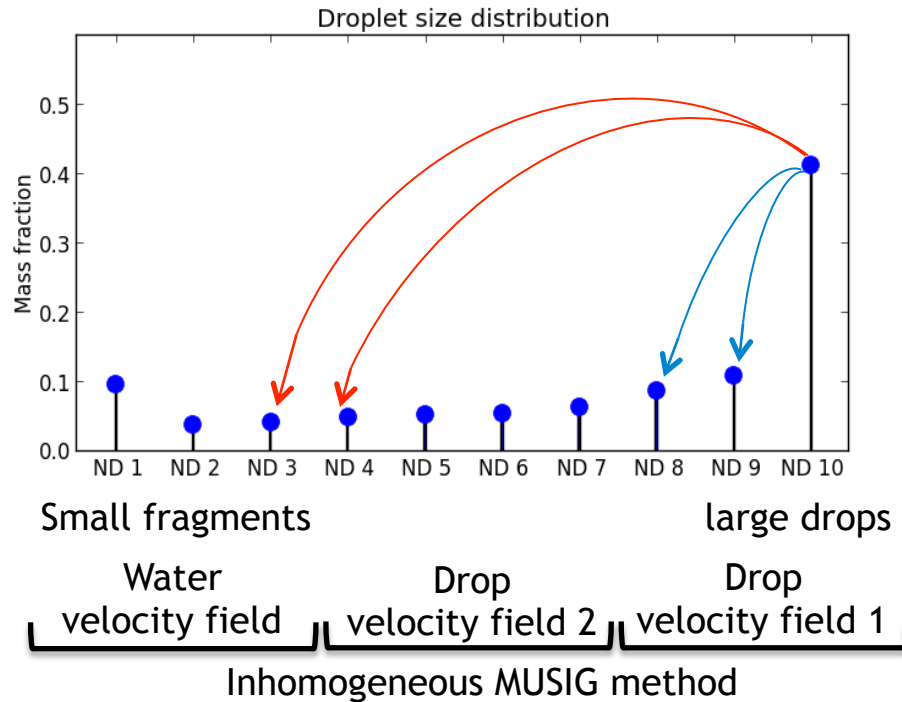
- Drop breakup
  - when the Weber number > critical value
- Drop fragmentation models
  - shear breakup regime
- Fragmentation ends in
  - 4 to 6 characteristic Ranger and Nicolls time



$$\tau \downarrow d = D \downarrow d / \Delta V \downarrow d c$$
$$\sqrt{\rho \downarrow d / \rho \downarrow c}$$

- Low Ohnesorge number
- No solidification

# Dispersed phase modelling in MC3D



Drop fragmentation rate

$$\Gamma_{frag,drop \rightarrow drop} = \alpha_d \rho_d c_{frag} \frac{\Delta V_{dc}}{D_d} \sqrt{\frac{\rho_c}{\rho_d}}$$

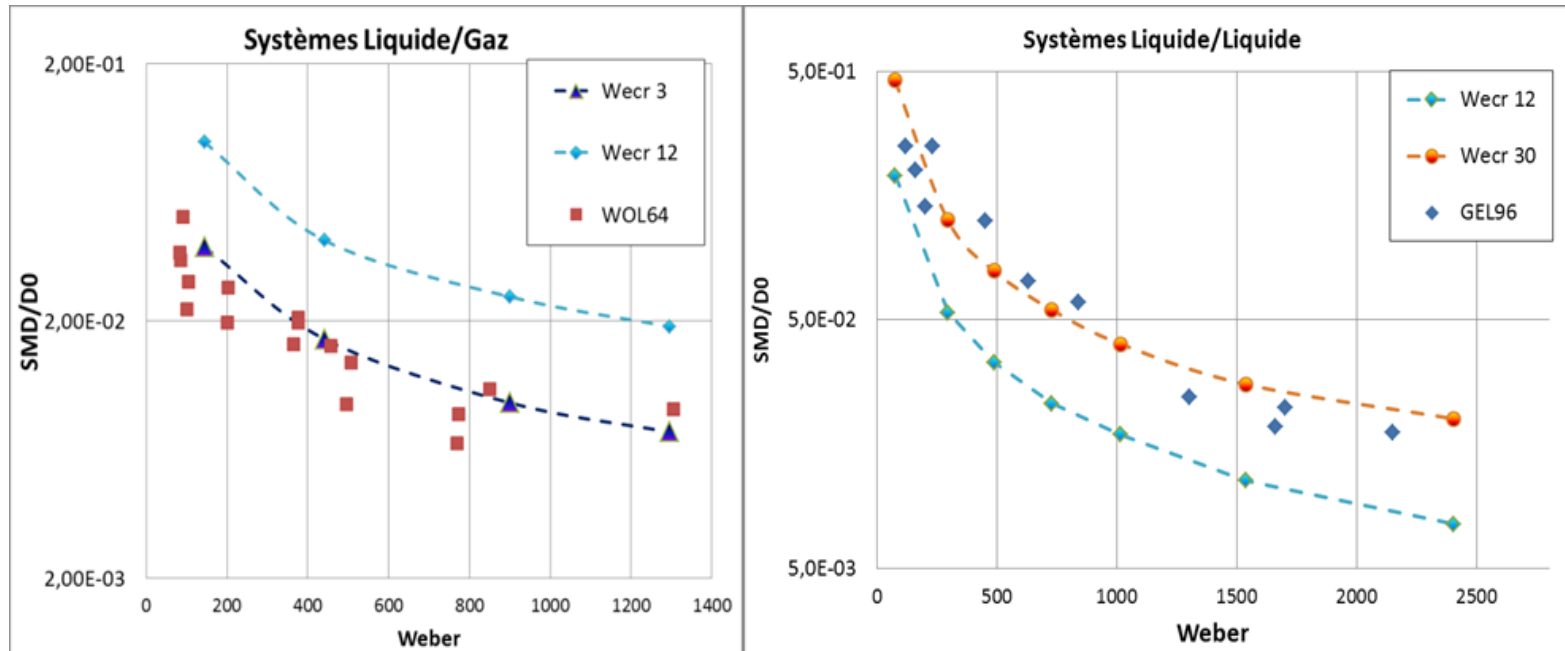
Generated fragment size

$$d_{daughter} = \frac{We_{ch} \sigma}{\rho_c (\Delta V_{dc})^2}$$

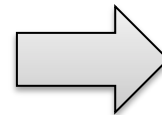
$$We_{ch} = Constant$$

Best results using a constant characteristic Weber number

# Drop breakup validation



- Different droplet size coefficient values for liquid/gas and liquid/liquid environments.
- Same fragmentation rate for L/L and L/G cases.
- Model is still too much user-dependent

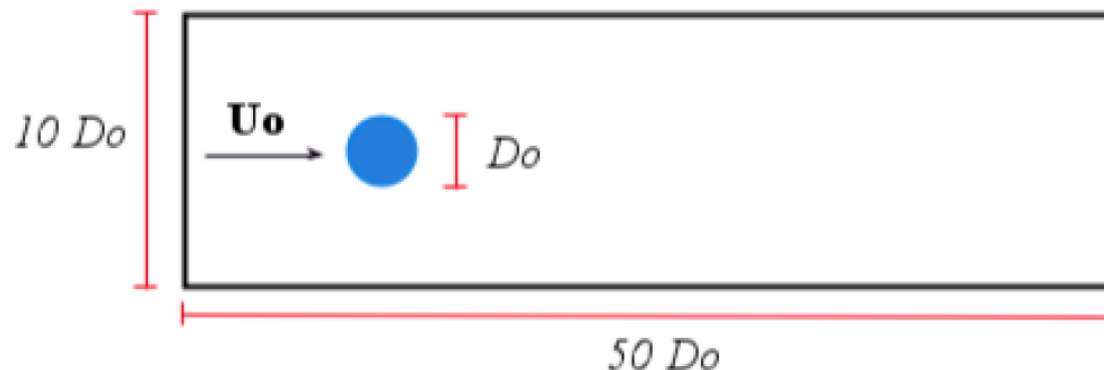
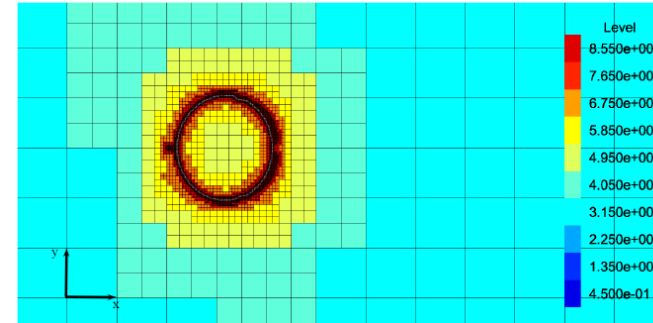


Improve analysis of fragmentation process

- Difference between L/L and L/G
- Influence of physical properties
- Drag coefficient during breakup

# Simulation of drop breakup using Gerris

- Why gerris???
  - Adaptive mesh refinement (AMR)
  - Parallel calculations / Fast calculation time
  - Previous studies of drop breakup performed with this CFD code
  - Internship with a Master student from UMPC (Azzara Annunziato)
  - Outputs for droplet size distribution
- Calculation parameters and domain
  - Liquid/Liquid (Gallium/Water) configuration (Surface tension of 0.7 N/m)
  - Weber number until 1300 => Range of FCI premixing stage



# Mesh criteria and simulation cases

- Based on a characteristic Weber number
  - Imposed minimum daughter size

$$\alpha = \frac{D_{probl}}{D_{daughter}} = \frac{We_{probl}}{We_{frag}}$$

- Ratio between mother drop and box length size

$$L = \beta \cdot D_0$$

- Gamma: Minimum number of cells per droplet

$$\gamma = \frac{D_{min}}{\Delta X_{min}} = 4.$$

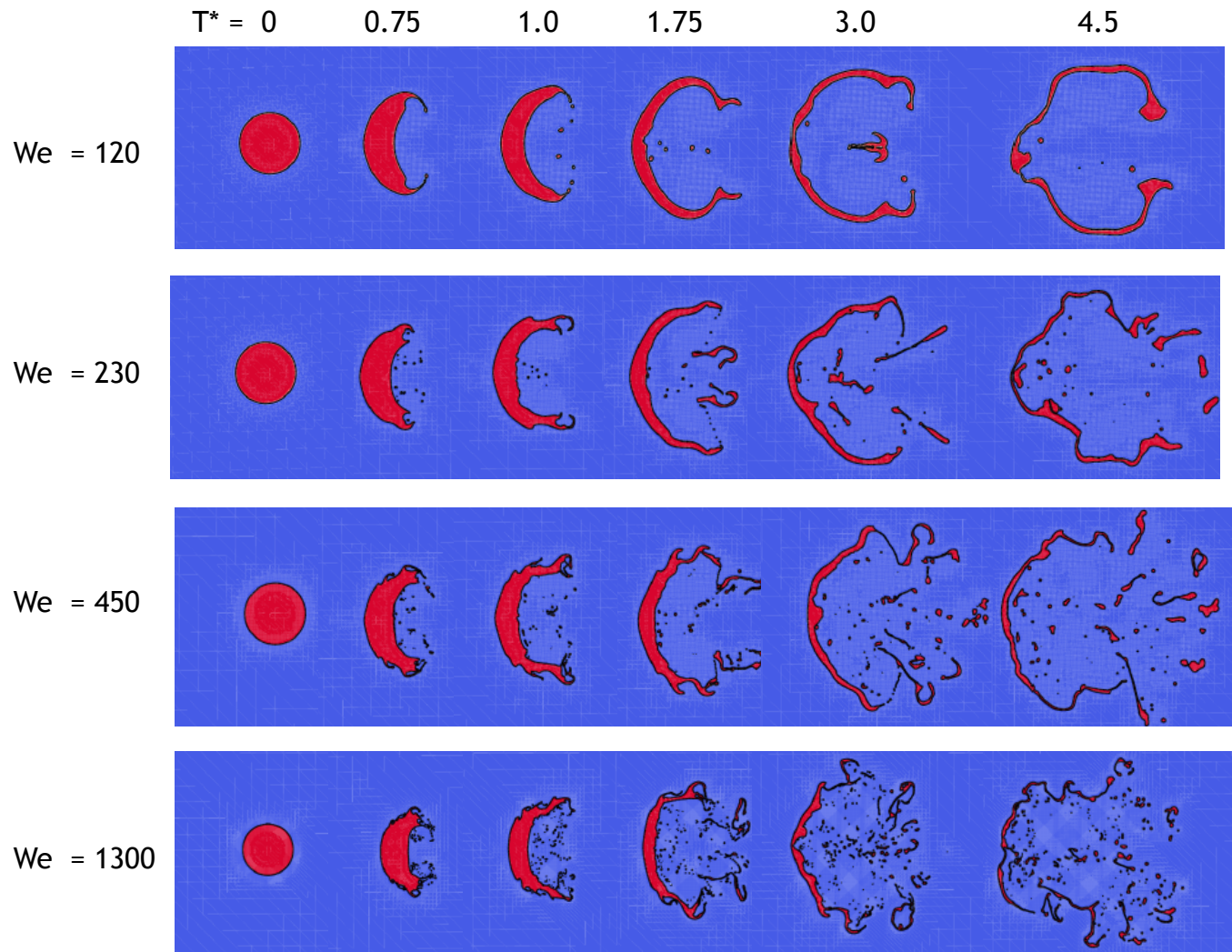
- Maximum refinement level

$$LEVEL = \frac{\ln(\alpha \cdot \beta \cdot \gamma)}{\ln 2}$$

Parameter	Symbol	Formula	Value
Density ratio	$\rho^*$	$\rho_d/\rho_c$	6.07
Viscosity ratio	$\mu^*$	$\mu_d/\mu_c$	1.6
Reynolds number	Re	$\frac{\rho_c D_0 u_0}{\mu_c}$	16 692–58 956
Weber number	We	$\frac{\rho_c D_0 u_0^2}{\sigma}$	120–1300

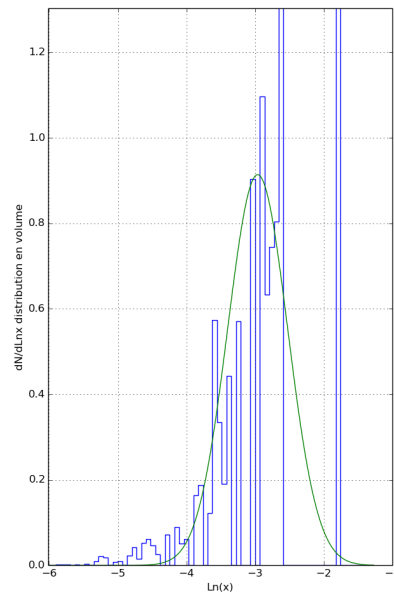
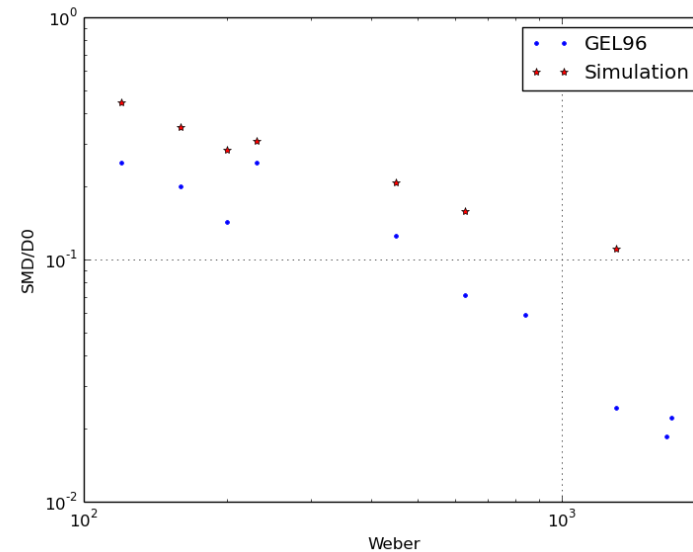
ID	$D_0$ (mm)	We	Re	$\tau$ (s)	$\alpha$	Level
a	3.3	120	16692	$1.61 \cdot 10^{-3}$	10.0	9
b	4.2	160	21744	$2.00 \cdot 10^{-3}$	13.3	9
c	4.2	230	26071	$1.67 \cdot 10^{-3}$	19.2	10
d	2.4	200	18377	$7.72 \cdot 10^{-4}$	16.7	10
e	2.8	450	29775	$6.49 \cdot 10^{-4}$	37.5	11
f	3.3	630	38246	$7.02 \cdot 10^{-4}$	52.5	11
g	3.8	1300	58956	$6.04 \cdot 10^{-4}$	108.3	12

# Some results (2D calculations)

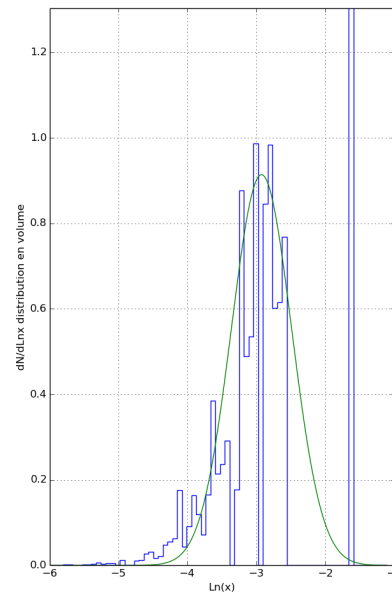


# Droplet size distribution

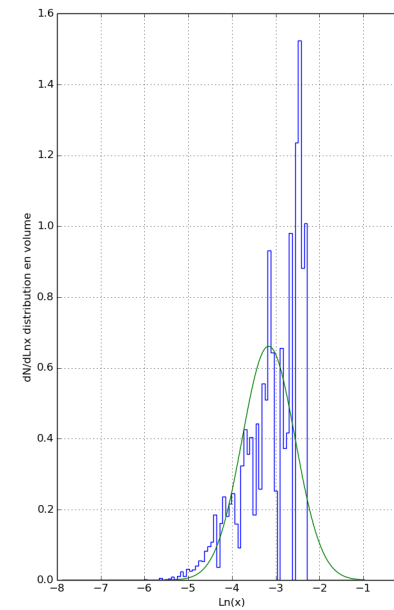
- Overestimation of the final Sauter Mean Diameter
- Results are not easily fitted with a log-normal distribution (no many simulations available to perform a statistical study)



We = 450  
D50/SMD = 1.1



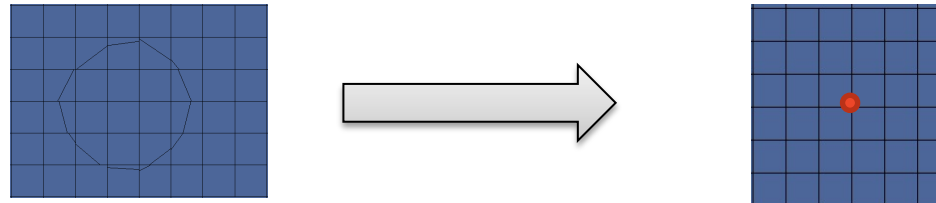
We = 630  
D50/SMD = 1.1



We = 1300  
D50/SMD = 1.2

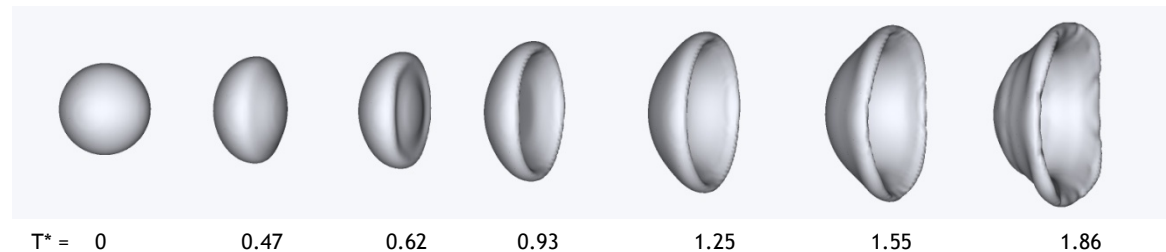
# How to improve simulations ???

- Convert VOF droplets into point-lagrangian particle when they become too small (They are generally stable => no further fragmentation)

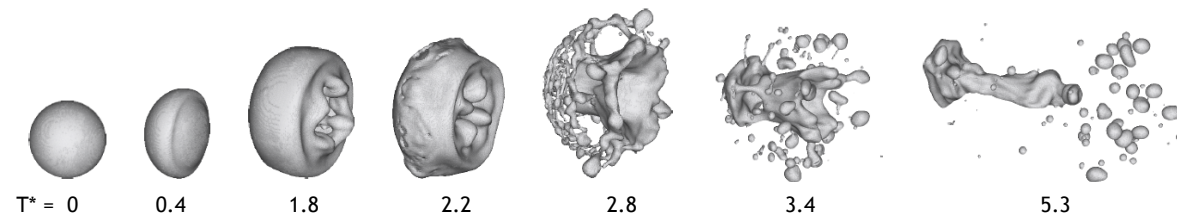


- Perform 3D simulations at different Weber numbers

We = 30



We = 120



- Better mesh refinement criteria (Higher refinement level)



# What's next???

- Introduce Lagrangian particules
- Perform data post-processing
  - Droplet size distribution
  - Droplet deformation
  - Drag coefficient
- Comprehension of droplet breakup in Liquid/Liquid systems and comparison with droplet breakup in FCI
  - Main mechanism for fragmentation
  - Effect of steam film (comparing drop entrainment)
- Deduce correlations or propose a new model to be implemented on MC3D
- Validation using the inhomogeneous MUSIG method

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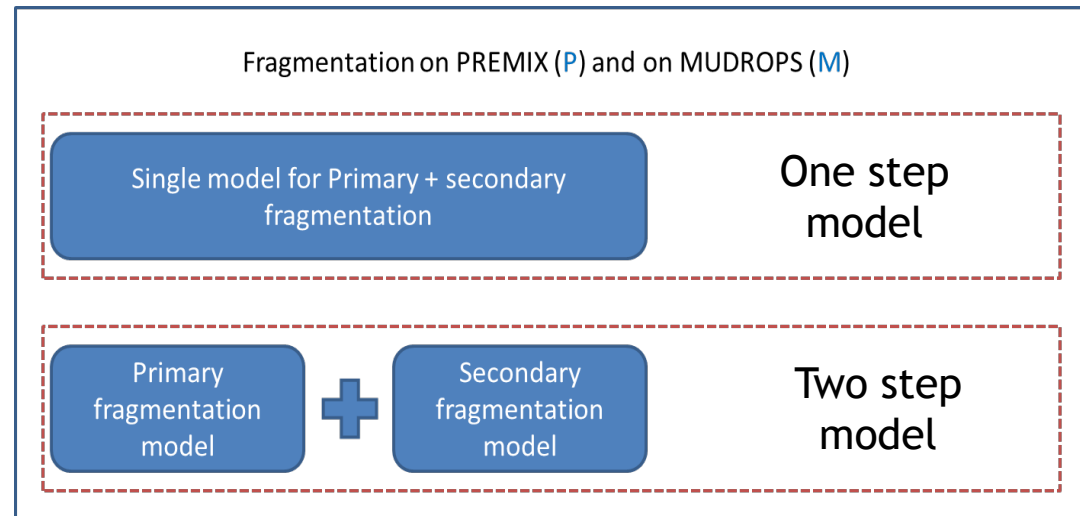
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Thank you

# Scope of work

## 1. Introduction, evaluation and analysis of fragmentation source terms

- ✓ Primary and secondary breakup
- ✓ coupled fragmentation models



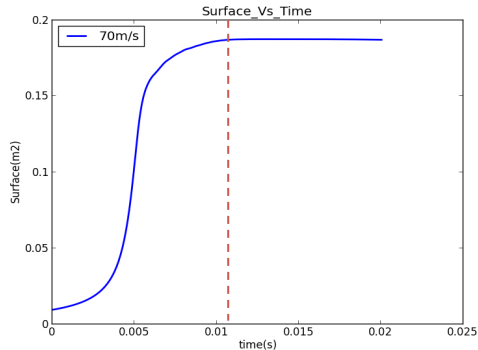
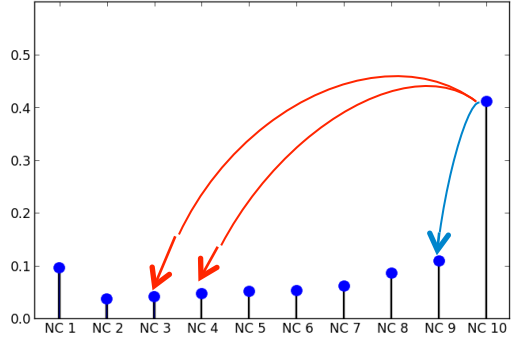
## 2. Introduction of Multi-Size Group (MUSIG) approach

- ✓ Homogeneous: One velocity field
- ✓ Inhomogeneous: Multi-velocity

Take into account polydisperse droplets and improve:

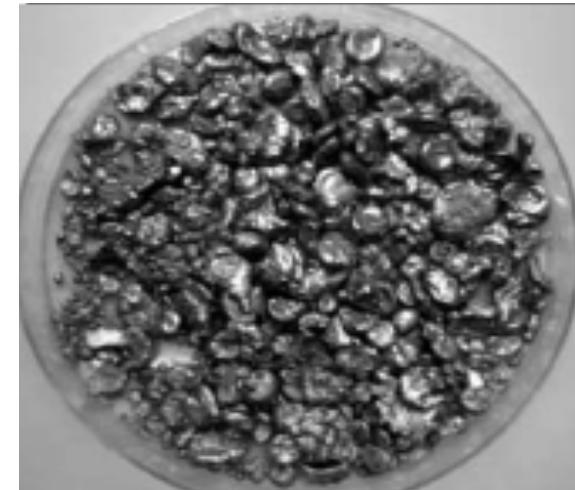
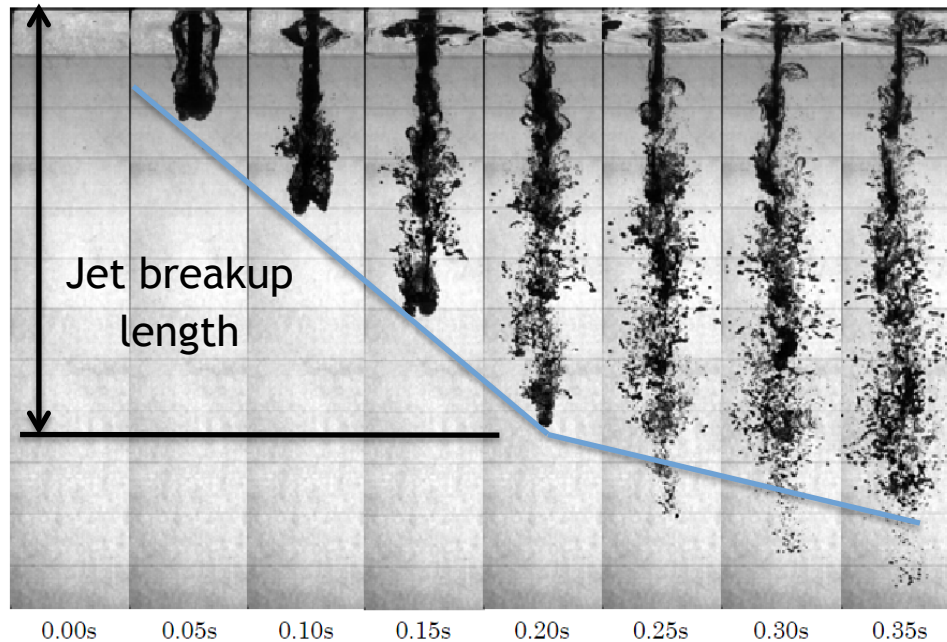
- Heat transfer
- Oxydation
- Solidification
- Breakup process

# Fragmentation source terms

	PREMEL (one droplet field + droplet area equation)	MUDROPS (Several droplet classes)
Primary fragmentation	<ul style="list-style-type: none"> <li>- Mass transfer from jet to droplet field</li> </ul> $\Gamma \downarrow frag \uparrow + , jet \rightarrow drop$ <ul style="list-style-type: none"> <li>- Droplet area creation</li> </ul> $\Gamma \downarrow A \uparrow + , jet \rightarrow drop$	<ul style="list-style-type: none"> <li>- Mass transfer from jet to several droplet classes</li> </ul> $\Gamma \downarrow frag \uparrow + , jet \rightarrow drop$
Secondary fragmentation	<ul style="list-style-type: none"> <li>- Droplet area creation</li> </ul> $\Gamma \downarrow A \uparrow + , drop \rightarrow drop$ 	<ul style="list-style-type: none"> <li>- Mass transfer between droplet classes</li> </ul> $\Gamma \downarrow frag \uparrow + , drop \rightarrow drop$ 

# Available experimental data / Validation

Liquid metal jet breakup experiments

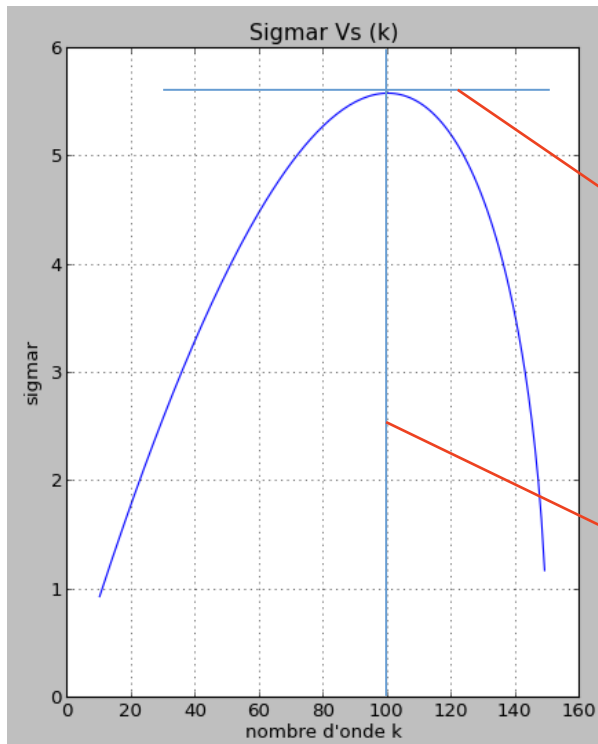
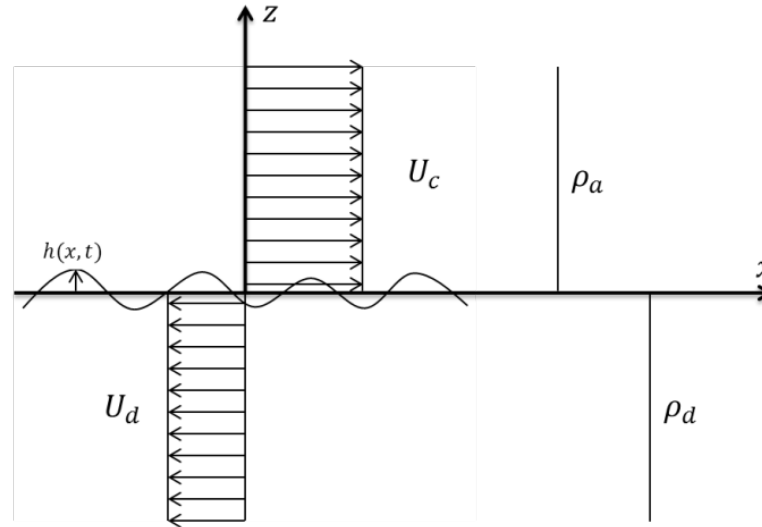


Solid fragments for a jet injection velocity of 2,10 m/s (ABE, et al., 2006)

- Final SMD
- Jet breakup length
- Droplet size distribution (for few experiments)

# Modelling hypothesis

Primary breakup related to the most unstable wave at the sheared interface



Instability growth rate  
 $\sigma \propto r, maximum$   
 $(c \propto i) =$

Proportional factor  
 $N \propto f$

Jet Fragmentation rate  
 $\Gamma \propto frag = N \propto f c \propto i$

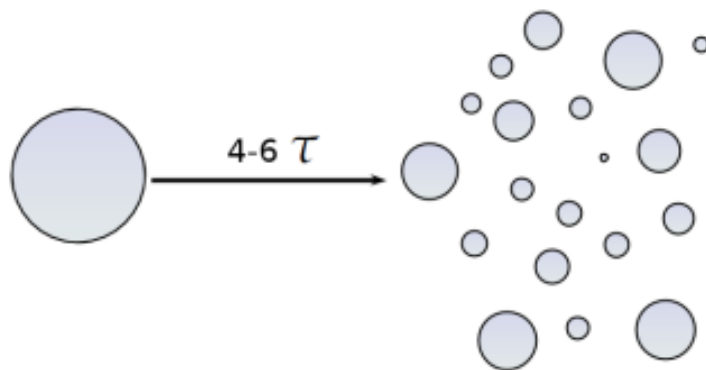
most unstable wavenumber corresponding to the maximum growth rate  
 $(\lambda \propto maximum = 2 \pi / (k \propto maximum))$

Proportional factor  
 $N \propto d$

Optimal size  
 $D \propto d, creatio$   
 $n = N \propto d$   
 $\lambda \propto m$

# Modelling hypothesis

- Drop breakup
  - when the Weber number > critical value
- Drop fragmentation models
  - shear breakup regime
- Fragmentation ends in
  - 4 to 6 characteristic Ranger and Nicolls time



$$\tau \downarrow d = D \downarrow d / \Delta V \downarrow d c$$
$$\sqrt{\rho \downarrow d / \rho \downarrow c}$$

- Low Ohnesorge number
- No solidification

# MUDROPS modelling

## Primary fragmentation

Droplet size distribution: Log-normal distribution characterized by:

$$SMD = N \int d^3 \pi \sigma (\rho_d + \rho_c) / \Delta V \int dc \int_2 \rho_d \rho_c \quad SMD/D_{0,50} = 1,2$$

Fragmentation rate:  $\Gamma_{frag, drop \rightarrow drop} = N \int f \Delta V \int dc \sqrt{1/3} \rho_d \rho_c / \rho_d + \rho_c$



# MUDROPS modelling

Secondary fragmentation

Drop fragmentation rate

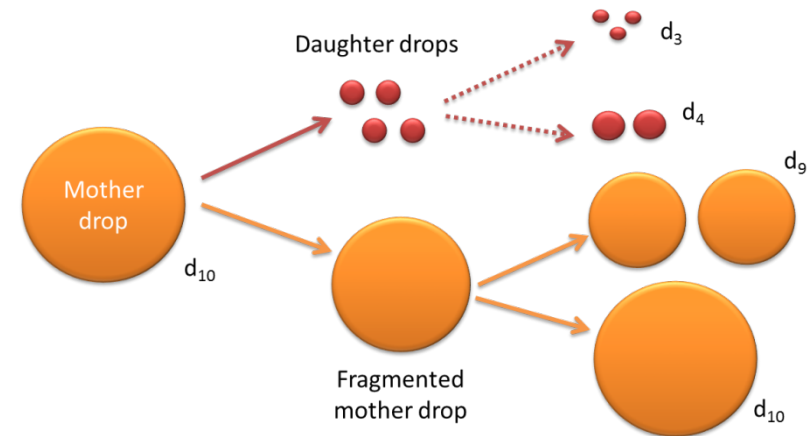
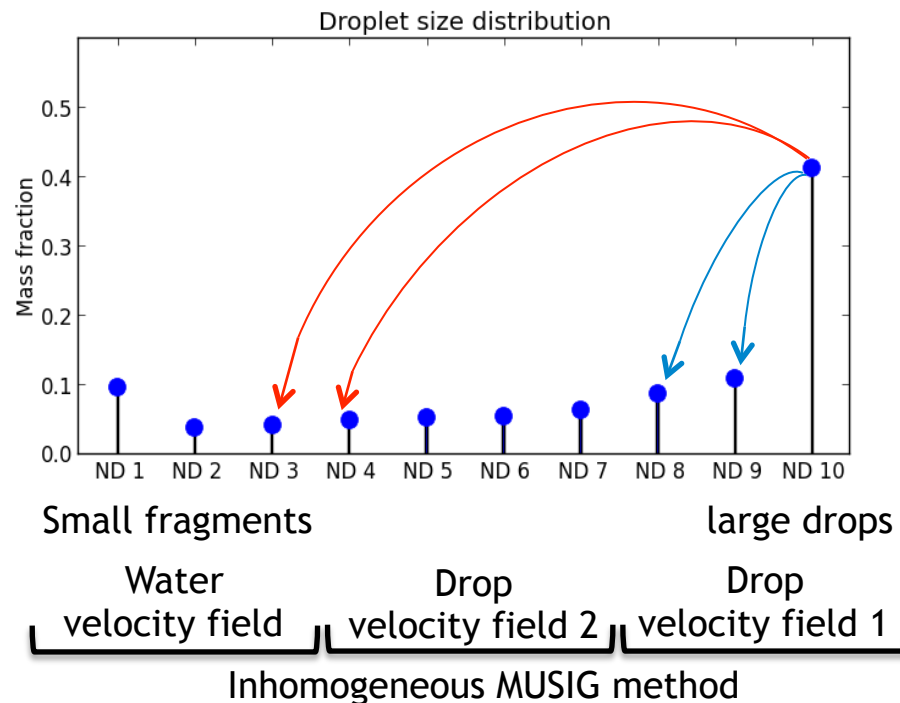
$$V \downarrow dc / D \downarrow d \sqrt{\rho \downarrow c / \rho \downarrow d}$$

$$\Gamma \downarrow frag, drop \rightarrow drop = \alpha \downarrow d \rho \downarrow d c \downarrow frag \Delta$$

Generated fragment size

$$d \downarrow daughter = We \downarrow ch \sigma / \rho \downarrow c (\Delta V \downarrow dc)^{1/2}$$

$$We \downarrow ch = Constant$$



# Jet breakup with MIF and MCF

- PIF model overestimates the final droplet SMD at low injection velocities (important effect of secondary breakup)
- PCF agrees with experimental data at different injection velocities. The simulation results follow a  $1/V$  function
- At high injection velocity, secondary breakup seems to have weak impact on the final droplet diameter.

# References

- [Gui09] Guildenbecher D. R, Lopez Rivera C, Sojka P. E: *Secondary Atomization*, Experiments in Fluids, Vol. 46, Issue 3 (2009), 371-402
- [Hsi92] Hsiang L. P, Faeth G. M: *Near-limit drop deformation and secondary breakup*, International Journal of Multiphase Flow, Vol. 18, N° 5 (1992), 635-652

# Hydrodynamic Secondary breakup: Drop size

Much more problematic:

- The constant Weber number assumption seems the most accurate (global shape)
- $We_{cr}$  differs for Liquid/Gas and Liquid/Liquid systems

- Constant characteristic Weber number

$$We_{\downarrow fragment} = We_{\downarrow critical} = Constant$$

- Classical Kelvin-Helmholtz instability

$$k = 2/3 (\Delta V_{\downarrow dc})^{1/2} \rho_{\downarrow d} \rho_{\downarrow c} / \sigma (\rho_{\downarrow d} + \rho_{\downarrow c}),$$

$$d_{\downarrow daughter} = C_{\downarrow 0} \lambda = C_{\downarrow 0} 2\pi/k$$

- Reitz et al. 1987

$$\lambda = 9.02 D_{\downarrow d} (1 + 0.45 \sqrt{Oh}) (1 + 0.4 T^{10.7}) /$$

$$(1 + 0.865 We^{1.67})^{10.6} \quad T = Oh \sqrt{We}$$

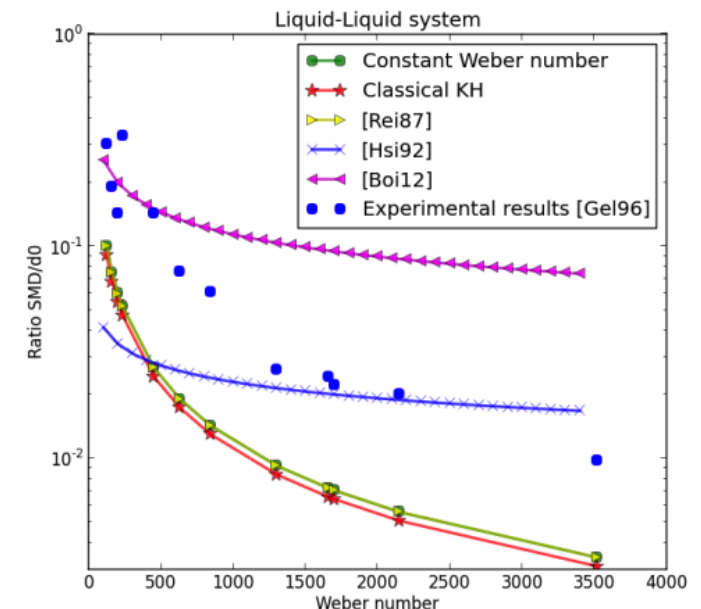
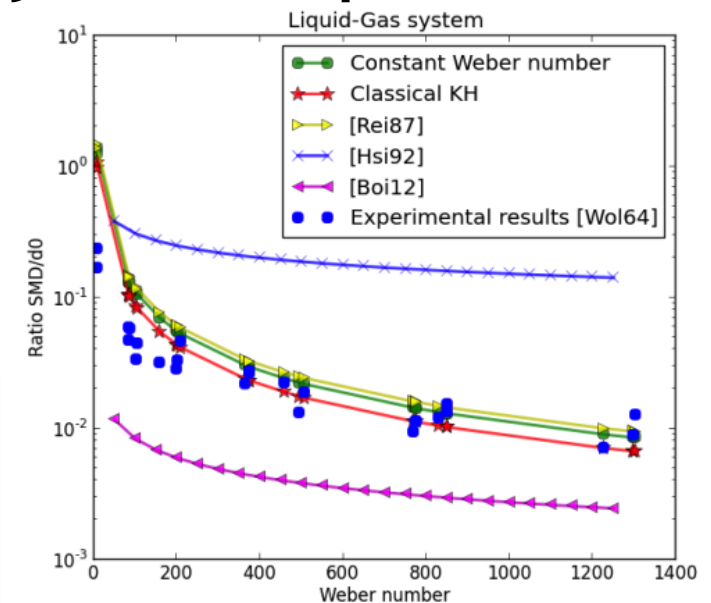
$$d_{\downarrow daughter} = 2B_{\downarrow 0} \lambda \quad (B_{\downarrow 0} = 0.61)$$

- Hsiang et al. 1992

$$We_{\downarrow ch} = C_{\downarrow s} (\rho_{\downarrow d} / \rho_{\downarrow c})^{1/4} [\mu_{\downarrow d} / \rho_{\downarrow d} D_{\downarrow d} \Delta$$

$$V_{\downarrow dc}]^{1/2} We_{\downarrow 0} \quad We_{\downarrow 0} = \rho_{\downarrow c} D_{\downarrow d} (\Delta V_{\downarrow dc})^{1/2} /$$

$\sigma$



## PREMIX APPLICATION

### Previous model

#### PREMEL

Dispersed field described by:

- One mass conservation equation
- A specific droplet area transport equation
- One momentum equation
- One energy equation

### New model

#### MUDROPS

Dispersed field described by:

- Several classes each one with its own mass conservation and energy equation
- One or multiple momentum equation
  - Homogeneous MUDROPS (One velocity field)
  - Heterogeneous/inhomogeneous MUDROPS (Three velocity fields)

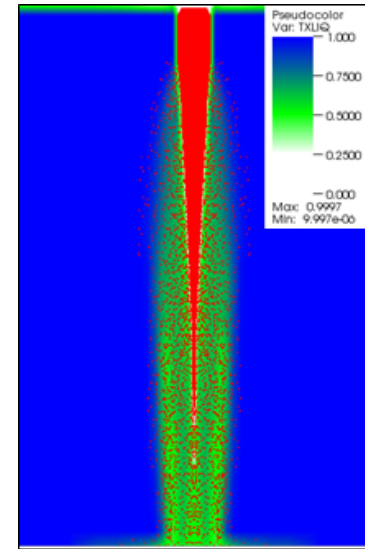
# CFD code MC3D

Primary breakup  
(Jet to drops)

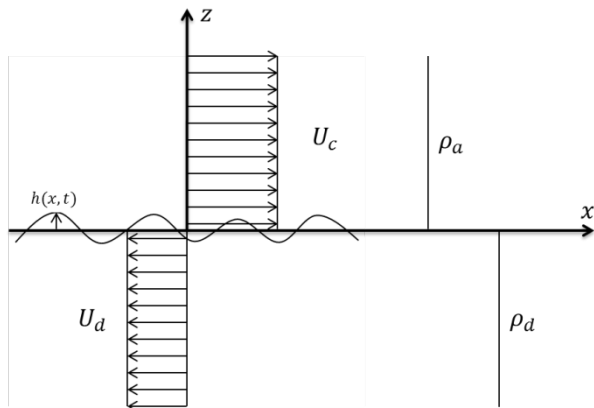
Secondary breakup  
(Drops to Drops)  
existing but not satisfactory

## Hypothesis for our work :

- Primary instability/fragmentation driven by large scale (integral scale)
- Secondary fragmentation driven by local conditions

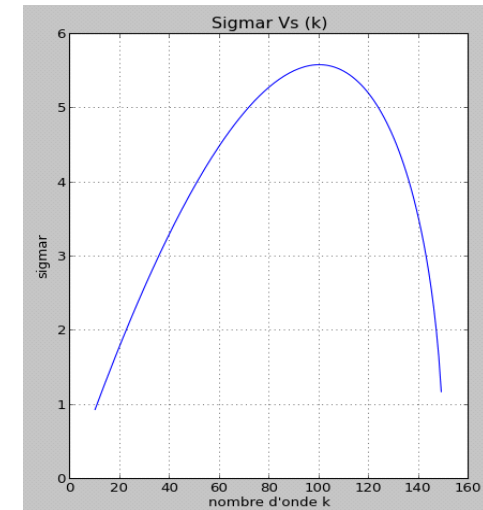


## Kelvin-Helmholtz model for primary jet fragmentation



$$\sigma_{kr} = k C_i = \sqrt{\rho_c \rho_d} \frac{k^2 (\Delta V)^2}{(\rho_c + \rho_d)^2} - \gamma \frac{k^3}{(\rho_c + \rho_d)}$$

- $C_i$  = characteristic velocity of perturbation growth
- $\Gamma_{frag} (primary) = N f C_i (N f > 0)$



# Hydrodynamic Secondary breakup

Hypothesis : Hydrodynamic forces cause the droplet to deform and to breakup  
(thermal aspects are neglected)

$$We = \rho v c D \Delta V / \sigma$$

$We < We_{cr}$  Stable drop, no secondary drop breakup

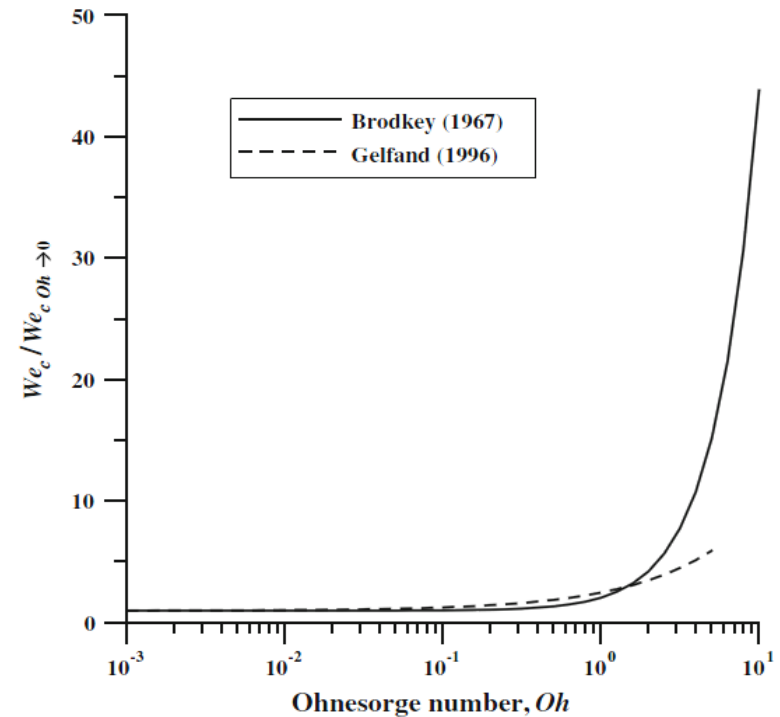
$We \geq We_{cr}$  Drop will breakup

$We_{cr}$  is usually a function of the Ohnesorge number

$$Oh = \mu / \sqrt{\rho D \sigma} = \sqrt{We} / Re$$

In our case,  $Oh \sim 10^{-3}$

Viscosity should have no impact.



Guildenbecher et al. 2009

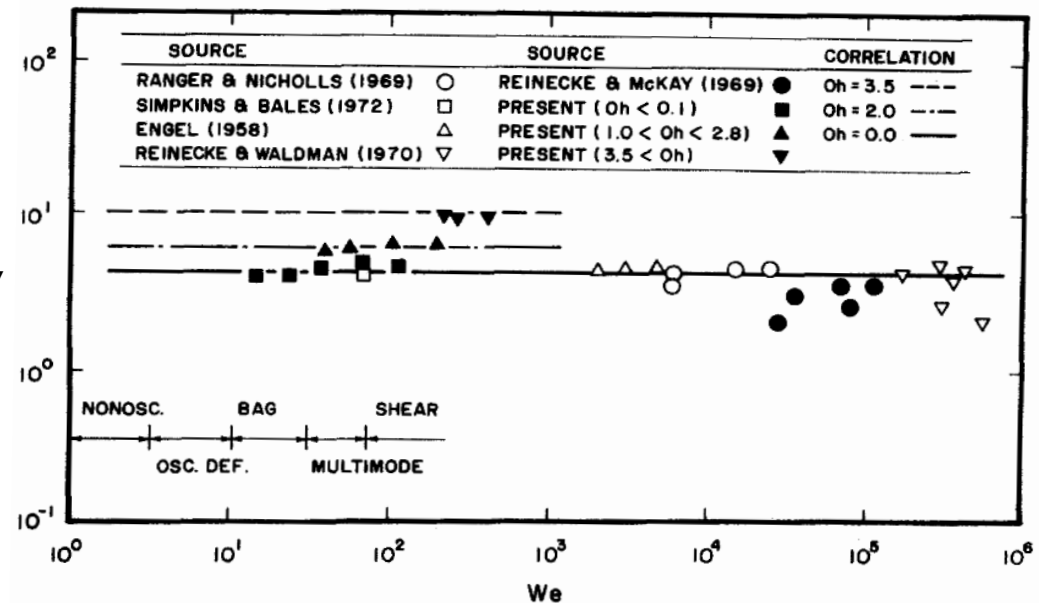
# Hydrodynamic Secondary breakup: Fragmentation rate

Drop breakup divided in two stages:

- Drop deformation (1 or 1,5  $\tau \downarrow d$ )
- Drop breakup (4 to 6  $\tau \downarrow d$ )

$$\tau \downarrow d = D \downarrow d / \Delta V \downarrow dc \sqrt{\rho \downarrow d / \rho \downarrow c}$$

$t / \tau \downarrow d$



Hsiang et al. 1992

- Total drop breakup time is nearly independent of the drop breakup regime
- Instantaneous volumetric drop fragmentation rate

$$\Gamma \downarrow frag = c \downarrow frag \text{ Drop Volume} / \tau \downarrow d$$



# Hydrodynamic Secondary breakup: Drop size

Much more problematic:

- The constant Weber number assumption seems the most accurate (global shape)
- $We_{\downarrow cr}$  differs for Liquid/Gas and Liquid/Liquid systems

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$$d_{\downarrow daughter} = C_{\downarrow 0} \lambda = C_{\downarrow 0} 2\pi/k$$

- Reitz et al. 1987

$$\lambda = 9.02 D_{\downarrow d} (1 + 0.45 \sqrt{Oh}) (1 + 0.4 T^{10.7}) /$$

$$(1 + 0.865 We^{1.67})^{10.6} \quad T = Oh \sqrt{We}$$

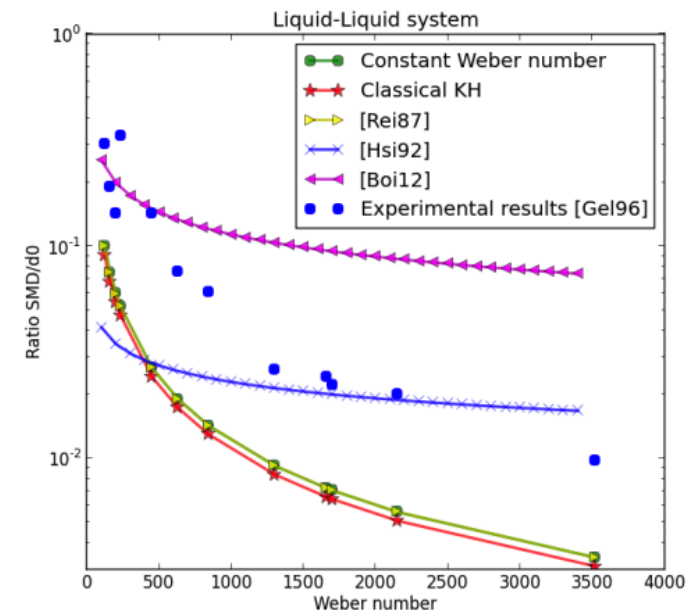
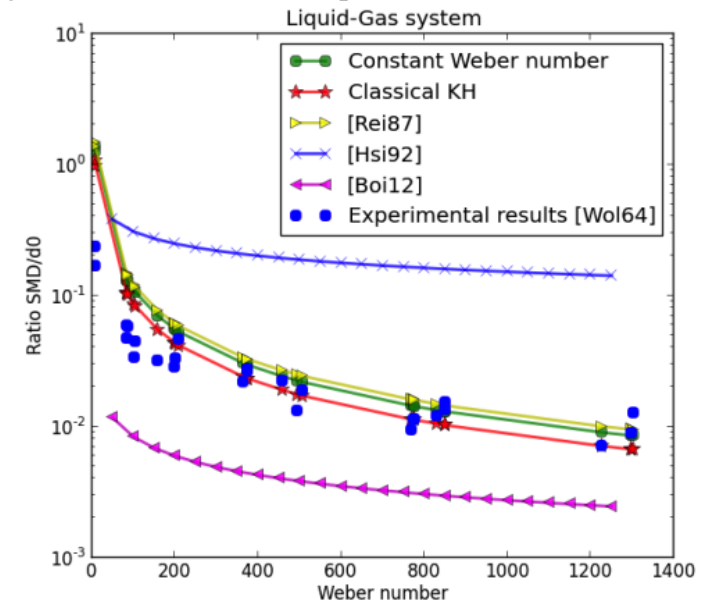
$$d_{\downarrow daughter} = 2B_{\downarrow 0} \lambda \quad (B_{\downarrow 0} = 0.61)$$

- Hsiang et al. 1992

$$We_{\downarrow ch} = C_{\downarrow s} (\rho_{\downarrow d} / \rho_{\downarrow c})^{1/4} [\mu_{\downarrow d} / \rho_{\downarrow d} D_{\downarrow d} \Delta$$

$$V_{\downarrow dc}]^{1/2} We_{\downarrow 0} \quad We_{\downarrow 0} = \rho_{\downarrow c} D_{\downarrow d} (\Delta V_{\downarrow dc})^{1/2} /$$

$\sigma$



# Hydrodynamic Secondary breakup

Drop fragmentation rate

$$\Gamma_{frag} = c_{frag} \alpha d \Delta V_{dc} / D d \sqrt{\rho d \rho c} = \alpha d \rho d c_{frag} \Delta V_{dc} / D d \sqrt{\rho c} / \rho d$$

Advantage: Each drop breaks up following local hydrodynamic conditions

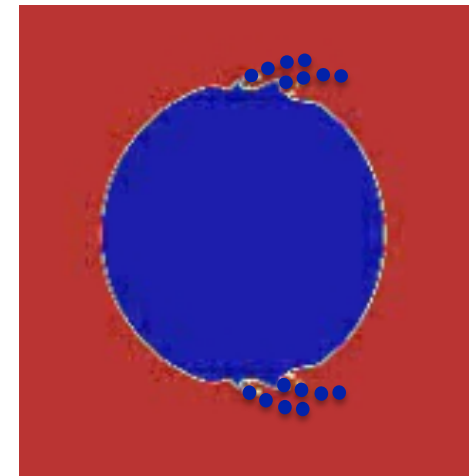
Generated fragment size

$$d_{daughter} = We_{ch} \sigma / \rho c (\Delta V_{dc})^{1/2}$$

$$We_{ch} = We_{critical} = Constant$$

Variation on the Mother droplet size (drop number conservation)

$$m_{final} = m_0 - \Gamma_{frag} \Delta t$$



Secondary Fragmentation scheme

# The MUSIG model

To limit the computational time, we must limit the number of velocity fields

- 1<sup>st</sup> approach : homogeneous
- 2<sup>nd</sup> approach : heterogenous with 3 fields, one being the water field : hydrodynamical equilibrium with water (no further fragmentation)

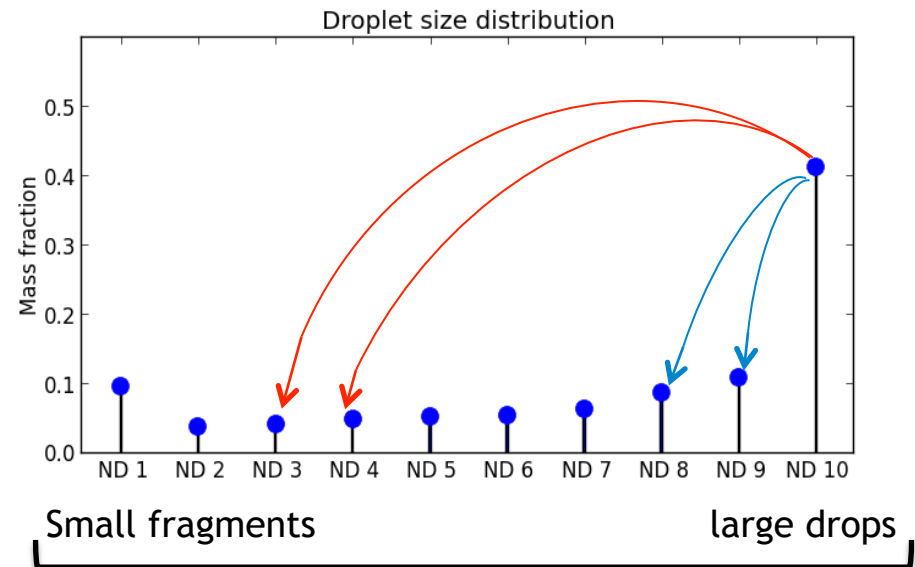
Mass transfert by stripping, generated fragments (e.g red lines)

$$\Gamma \downarrow D \downarrow d \rightarrow d \downarrow 1 = \Gamma \downarrow frag (d \downarrow 1 \ d \downarrow 2 - d \downarrow 1 \ d \downarrow daughter) / d \downarrow daughter (d \downarrow 2 - d \downarrow 1)$$

$$\Gamma \downarrow frag = \Gamma \downarrow D \downarrow d \rightarrow d \downarrow 1 + \Gamma \downarrow D \downarrow d \rightarrow d \downarrow 2$$

Mass transfert by mother drop mass depletion (e.g blue lines)

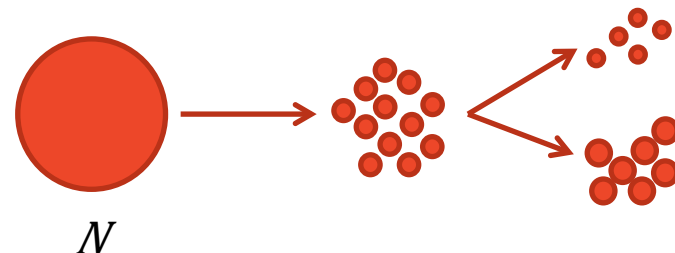
$$\Gamma \downarrow D \downarrow d \rightarrow d \downarrow 1 = (\alpha \downarrow d \ \rho \downarrow d / \Delta t - \Gamma \downarrow frag) (d \downarrow 1 \ d \downarrow 2 - d \downarrow 1 \ d \downarrow f) / d \downarrow f (d \downarrow 2 - d \downarrow 1)$$

$$\Gamma \downarrow D \downarrow d \rightarrow d \downarrow 2 = \Gamma \downarrow frag - \Gamma \downarrow D \downarrow d \rightarrow d \downarrow 1$$


Homogeneous MUSIG method

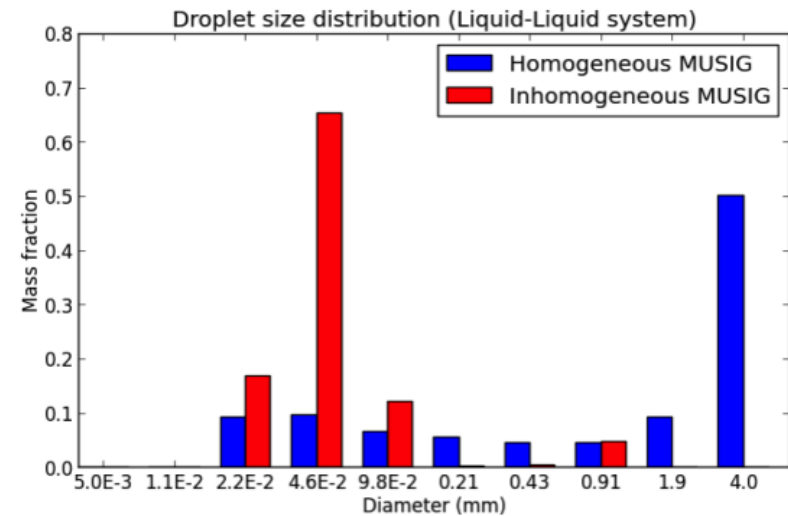
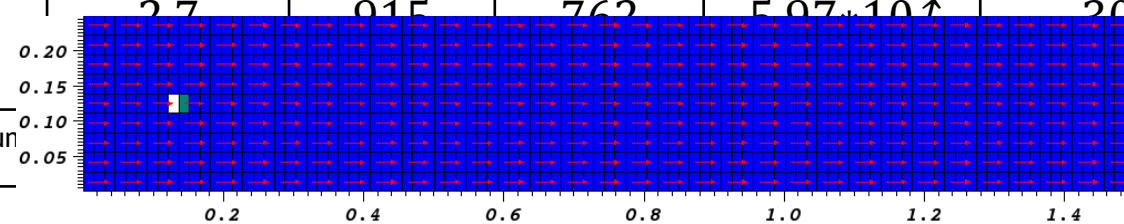


Inhomogeneous MUSIG method



# Validation : single drop fragmentation

Physical properties		Initial drop diameter (mm)	Drop Density $kg/m^3$	Density ratio	Dynamic Viscosity $Pa \cdot s$	Dynamic viscosity ratio	Surface Tension $N/m$
Liquid/Gas	Bis	2.7	915	762	$5.07 \cdot 10^{-4}$	200	0.0276
Liquid/Liquid	Gallium						0.7036

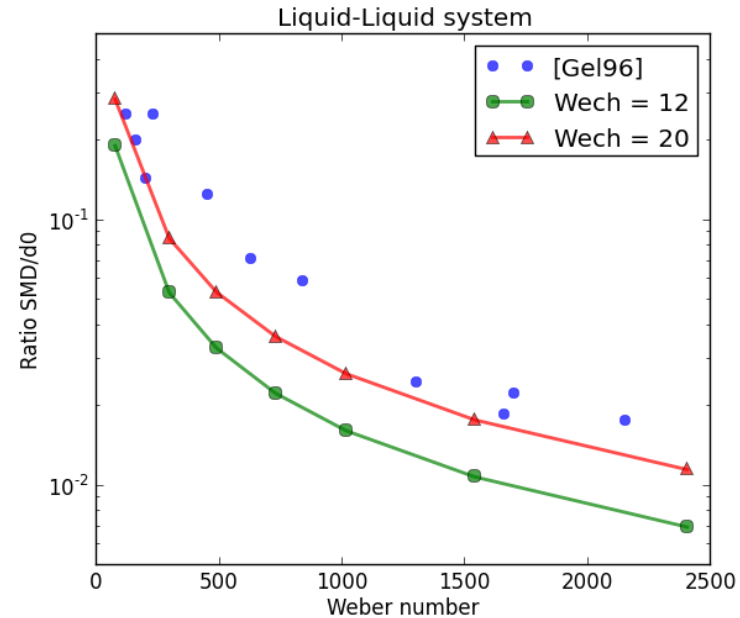
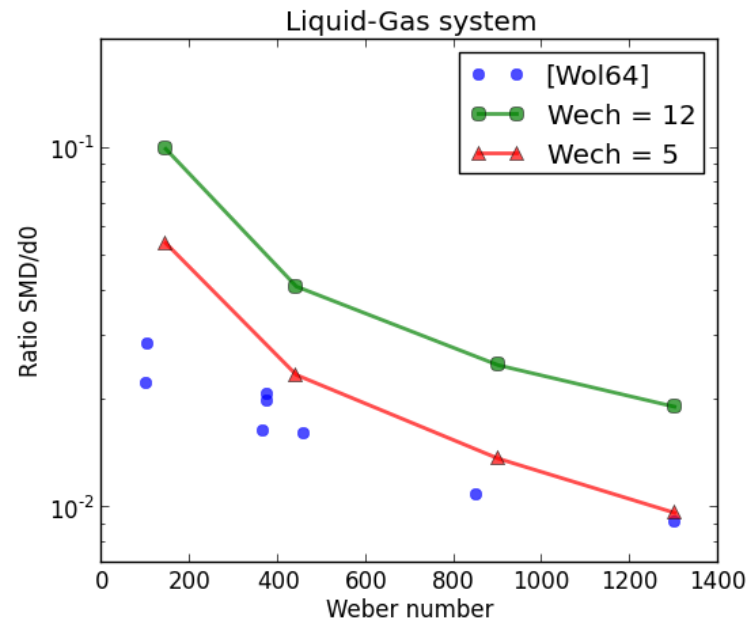


$t \gg 5\tau \downarrow d$

Homogenous MUSIG method not satisfactory because a large fraction of large drops are not fragmented.

- o Due to a too important entrainment with the small fragments

# Validation : single drop fragmentation



Typical characteristic Weber number:  $We_{ch} = 12$

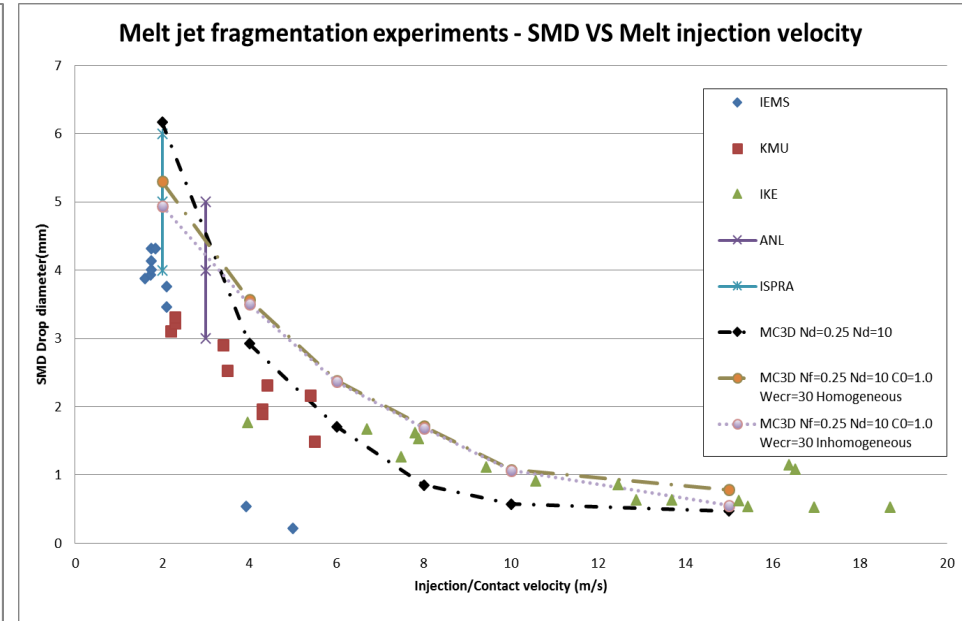
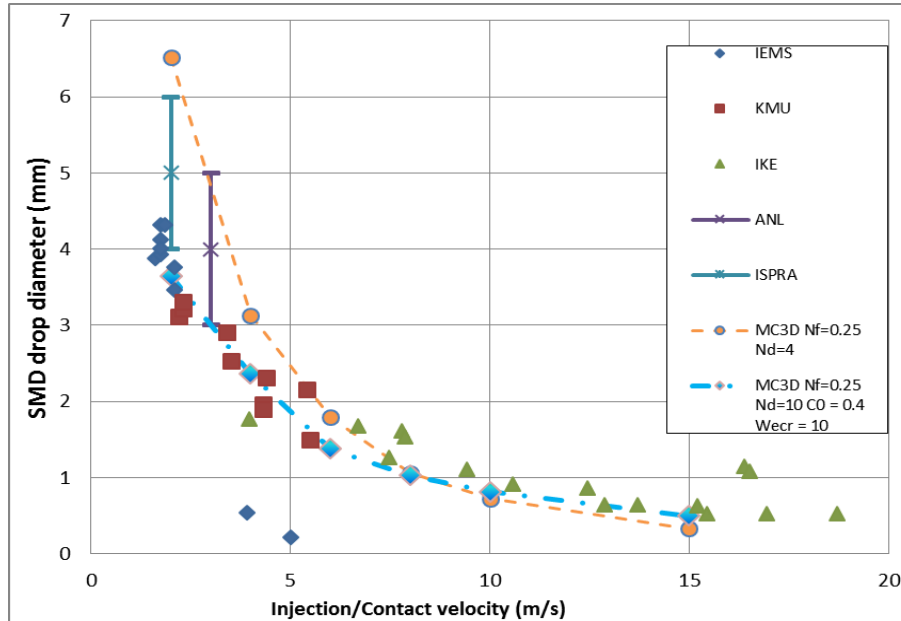
Correct general tendency but different characteristic Weber number for the best fit with experimental results:

- o Liquid/Gas systems  $We_{ch} = 5$
- o Liquid/Liquid systems  $We_{ch} = 20$

Possible causes:

- o Drop entrainment: Present drag law  $C_{\downarrow d} = \max(\min(0,5 ; 2d/3 \sqrt{g(\rho_{\downarrow d} - \rho_{\downarrow c})/\sigma} ); 24/Re (1 + 0,1 Re^{10,75} ) )$
- o Drop stretching (Deformation) : liquid is entrained before fragmentation

# Liquid metal jet breakup



One step fragmentation

$$N \downarrow d = 4$$

$$N \downarrow f = 0,25$$

Two step fragmentation

Primary fragmentation

$$N \downarrow d = 10$$

$$N \downarrow f = 0,25$$

Secondary fragmentation

$$C \downarrow 0 = 1,0$$

$$We \downarrow cr = 30$$

# Conclusions and Perspectives

- ✓ A secondary fragmentation model was introduced in the MC3D code, based on a MUSIG approach.
- ✓ The homogenous approach is not appropriate for liquid/liquid systems
- ✓ Use of 3 velocity field gives satisfactory results in first analysis

## Continuation / Improvements:

1. Improve analysis of fragmentation processes (with a simulation tool in particular)
  - difference L/G and L/L ?
  - impact of viscosity ?
2. Analysis of drag coefficient during fragmentation
3. Influence of multiphase environments for application to FCI
4. New experimental setup for validation of melt fragmentation process

# References

- [Gui09] Guildenbecher D. R, Lopez Rivera C, Sojka P. E: *Secondary Atomization*, Experiments in Fluids, Vol. 46, Issue 3 (2009), 371-402
- [Hsi92] Hsiang L. P, Faeth G. M: *Near-limit drop deformation and secondary breakup*, International Journal of Multiphase Flow, Vol. 18, N° 5 (1992), 635-652