*11th June 2015*
*DIERS Meeting Düsseldorf, DE*

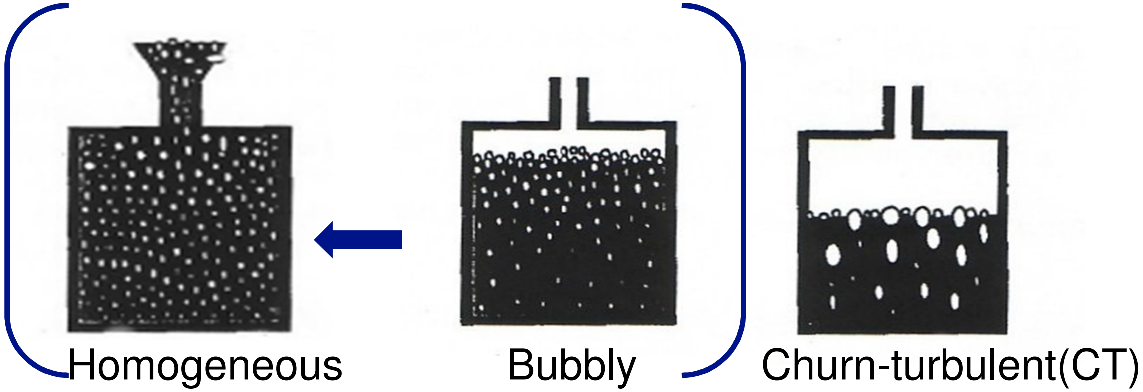
# Vapor runaway reaction: 1-φ or 2-φ vent flow?

**Presented by** **Jie XU**

**Under the supervision of:**
Jean-Pierre Bigot
Ana Cameirao
Jean-Michel Herri
Aymeric Guinaudeau
Wassila Benaissa
Sébastien Righini

# Introduction

- **To predict venting flow nature (1- or 2-phase), we need to model the disengagement in the reactor.**

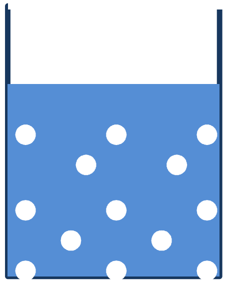


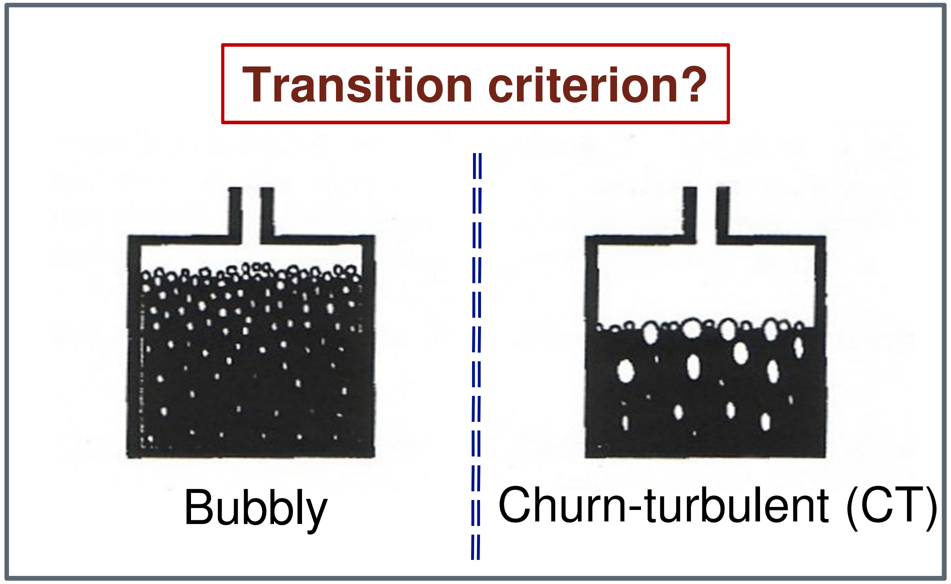

- **June 2014: beginning of my PhD work – EDUG Buxton,UK**
  - Jean-Pierre Bigot: why is disengagement not more taken into account?
  - Answers obtained from the attendants:
    - Models were already developed.
    - Several companies use these models.

*J. Etchells and J. Wilday, Workbook for Chemical Reactor Relief System Sizing.1998*
*Fai 83-27,A summary of Multiphase flow methods, 1983*

# Major issues

**Hypothesis:**
**uniform vapor generation in the bulk.**






1. **How to predict the reactor flow pattern?**
2. **Does vapor generates uniformly in the bulk ?**

# Summary

Bubbly – Churn-turbulent transition criterion

Vapor generation: uniform in the bulk ?

Perspectives

# 1st part

**Bubbly – Churn-turbulent transition criterion**

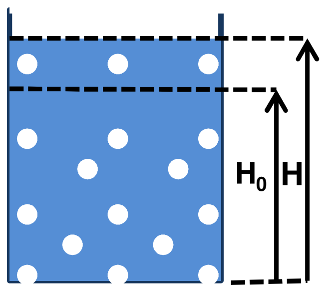
Vapor generation: uniform in the bulk ?

Perspectives

# Bubbly – churn turbulent transition criterion

- **α (void fraction)**
  - FAI 83/27, $\alpha_{transition}$ = 0.15 – 0.25, sometimes until 0.5.
  - Large pipes gas injection research, $\alpha_{transition} \approx 0.3$.

- **α (void fraction) & $d_b$ (bubble diameter)**
  - Map of Zuber & Hench experiments (1962).

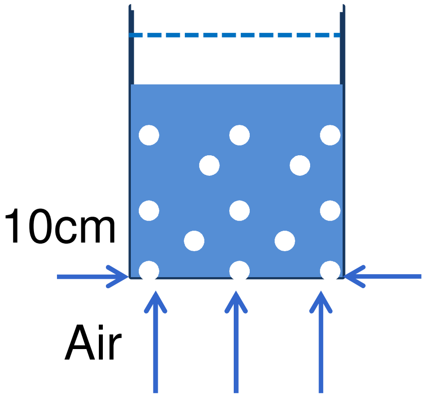



Void fraction: $\alpha = \frac{H}{H_0} - 1$

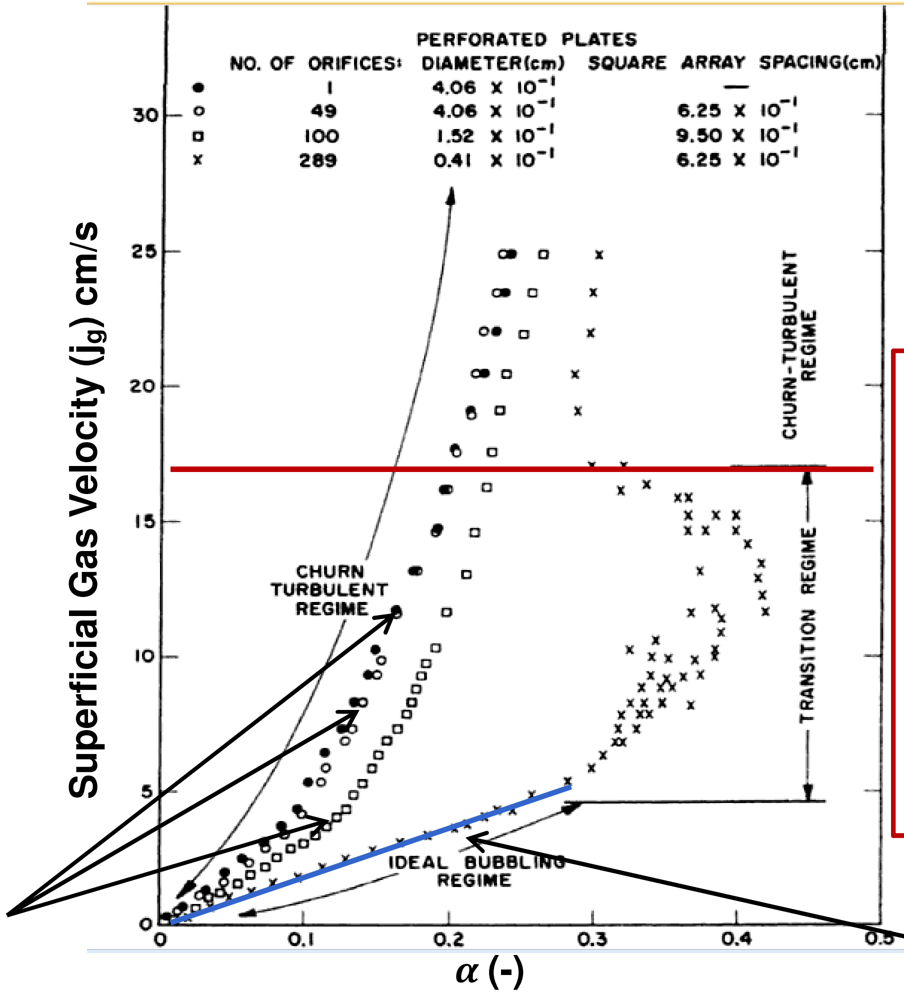
*Zuber N. and Hench .J, General Electric Co., Schenectady, NY, 62 GL 100, 1962.*
*J. P. Schlegel et al., Nucl. Eng. Des., vol. 239, no. 12, pp. 2864–2874, December 2009.*

# Bubbly – churn turbulent transition criterion

- Zuber & Hench experiments (1962)




$$j_g = \frac{Gas\ flow\ rate}{Section\ Area}$$




Large bubbles

Small bubbles

**Churn-turbulent ascertained , if**
- $j_g > 17cm/s$
  or
- $d_b$ is large enough

- **Influence of initial bubble size on the reactor flow pattern?**
- **Is bubbly a quite rare occurrence during a runaway reaction?**

*Zuber N. and Hench .J, General Electric Co., Schenectady, NY, 62 GL 100, 1962.*

# Discussion: flow pattern prediction

- **For vent sizing,**

Bubbly

- Conservative
- Large vent area

Churn-turbulent (CT)

- More efficient depressurization
- Smaller vent area

$\alpha \downarrow \rightarrow$ Vent size $\downarrow$

Sufficient condition to be defined

# Flow pattern determination proposal

Start

$j_g > 17$ cm/s

Yes → **Churn-turbulent flow**

- $j_g > 17$ cm/s ?
- Probably the more frequent case during a runaway.
- Easy to determine from adiabatic experiments.

No ↓

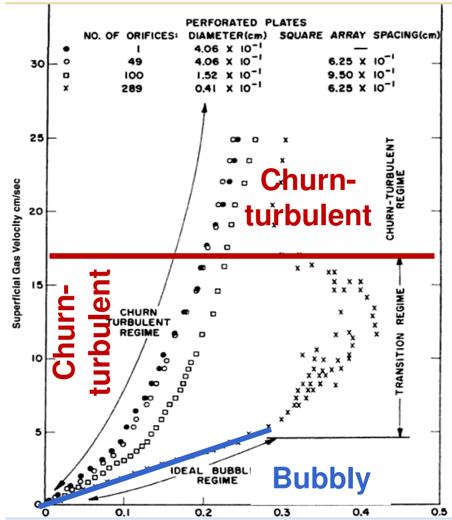
$d_b >$ distortion threshold

Yes → **Churn-turbulent flow**

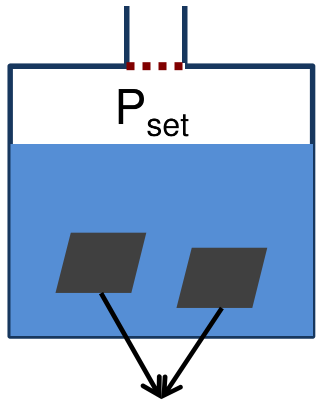
- Constant pressure ($P_{set}$) small scale visualization to see the $d_b$ when bubbles detach.

No ↓

**Bubbly flow**




Possible test :

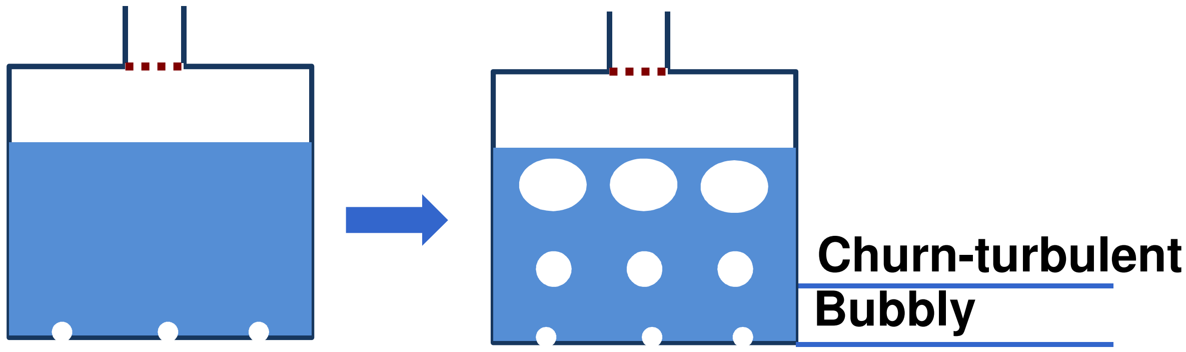



Pieces of reactor and instrument materials

**Do you agree with this determination?**

# Bubbly – churn turbulent transition criterion

- Bubbles rise up and grow.
- Possible flow pattern change.




**Useful to model for this flow pattern transition?**

# Bubbly – churn turbulent transition criterion

- **α (void fraction)**
  - FAI 83/27, $\alpha_{transition}$ = 0.15 – 0.25, sometimes until 0.5.
  - Large pipes gas injection research, $\alpha_{transition} \approx 0.3$.
- **α (void fraction) & $d_b$ (bubble diameter)**
  - Map of Zuber & Hench experiments (1962).
- **Viscosity**
  - DIERS Project Manual

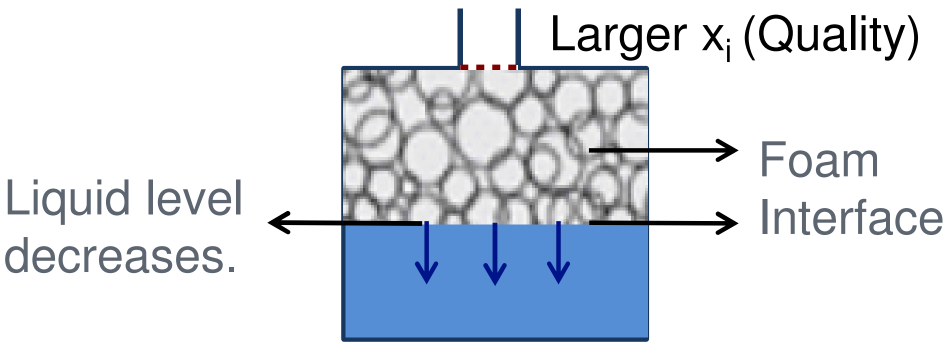
| Disengagement Regime | Viscosity | Foaming Tendency |
|---|---|---|
| Churn-turbulent | < 100 mPa.s | no |
| Bubbly | ≥ 100 mPa.s | no |
| Homogeneous | - | yes |

**Linked to another definition of bubbly flow pattern?**

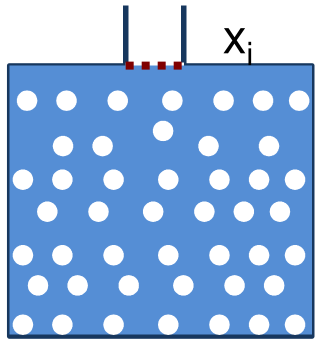
*Zuber N. and Hench .J, General Electric Co., Schenectady, NY, 62 GL 100, 1962.*
*J. P. Schlegel et al., Nucl. Eng. Des., vol. 239, no. 12, pp. 2864–2874, December 2009.*

# Foamy behavior: homogeneous model?

- **Bell & Morris Visualization**
  - Water + surfactant
  - $P_{set}$ = 5 bar
  - T = 110°C
  - $V_{reactor}$ = 13L




Foamy behavior




Homogeneous model

**Correct to use "homogeneous" for "foamy" ?**


*K. Bell and S. D. Morris, J. Loss Prev. Process Ind., vol. 5, no. 3, pp. 160–164, 1992*

# $2^{nd}$ part

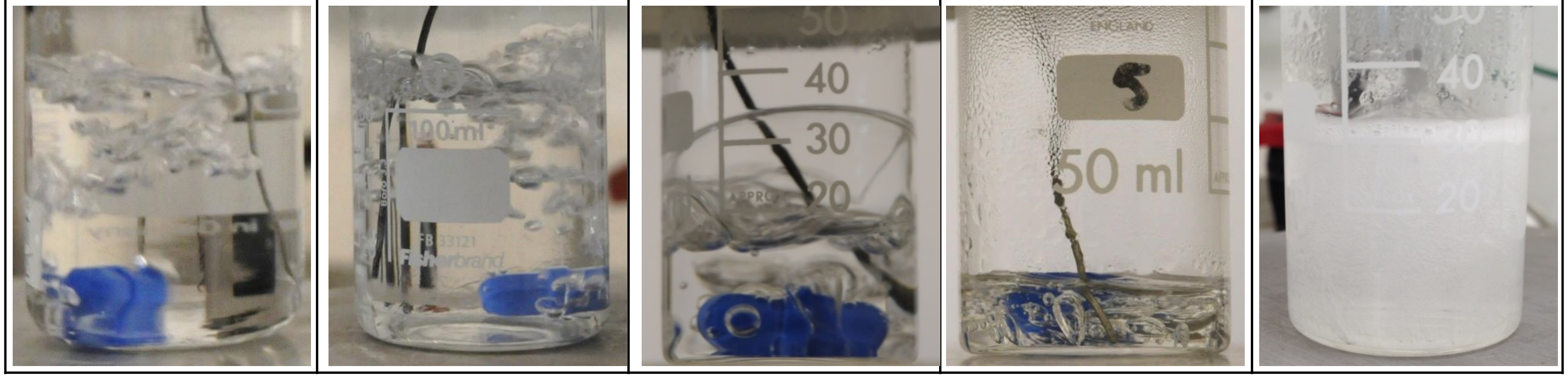
Bubbly – Churn-turbulent transition criterion

**Vapor generation: uniform in the bulk ?**

Perspectives

# Preliminary visualization in pool condition

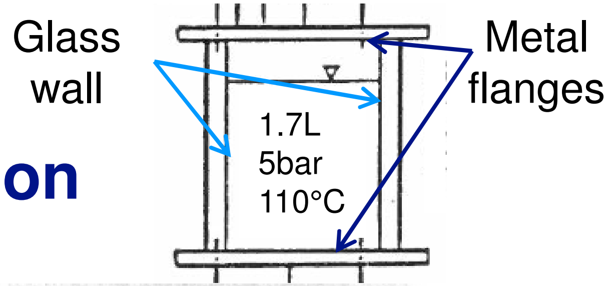
| Esterification | Hydrolysis | Water + PAA | AA --- PAA 25% | $H_2O_2$ decomposition |
|---|---|---|---|---|




- **Bubbles nucleate at the interfaces: reactor walls, magnetic stirrer,** except perhaps for $H_2O_2$ decomposition.

- **Bubbles are already large when they leave from their nucleation sites,** except for $H_2O_2$ decomposition.


MINES Saint-Étienne




# Friedel & Wehmeier: Esterification


- Bubbles nucleate at the rough cold metallic surfaces and one defect on the left glass wall.
- Bubbles are already large when they leave from their nucleation sites.

- **Interfacial , often large bubble generation. Do you agree?**
- **Any other paper dealing with runaway reaction visualization?**
- **Some visualization during the large-scale DIERS experiments?**

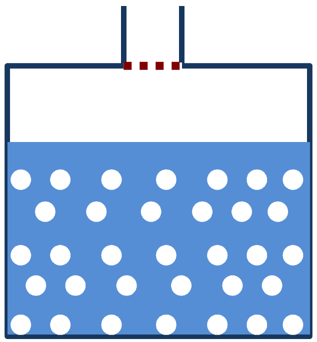
*Guido Wehmeier, PhD dessetation 170 94.*

# Discussion: uniform bulk vapor generation?

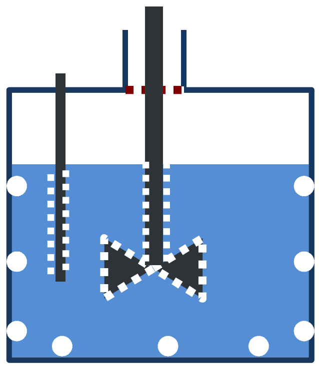
DIERS – FAI1983-27
Uniform bulk vapor generation

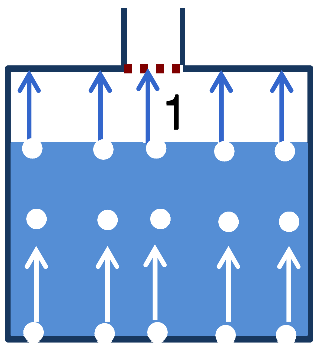
Compatible?

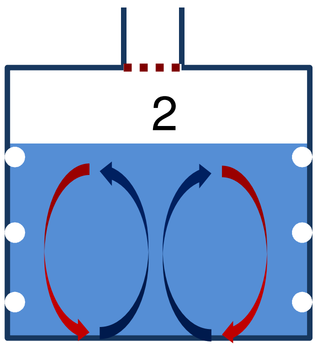
Interfacial bubble nucleation



Interfacial area (bubbles) available almost everywhere during a runaway reaction.





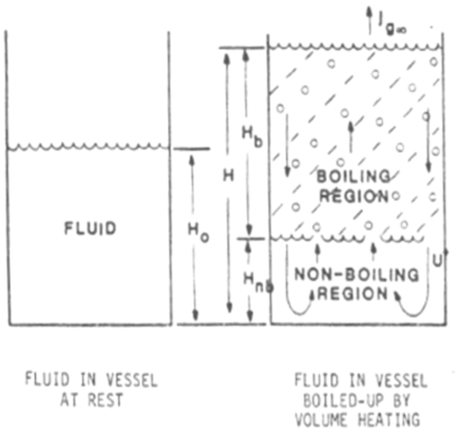

1. Enough bubbles detach from the bottom nuclei sites to compensate for the bubbles which are disengaging. (more frequent)
2. Convection brings vertical wall bubbles to the whole bulk.

**Do you think this understanding is correct?**

# Discussion: uniform bulk vapor generation?

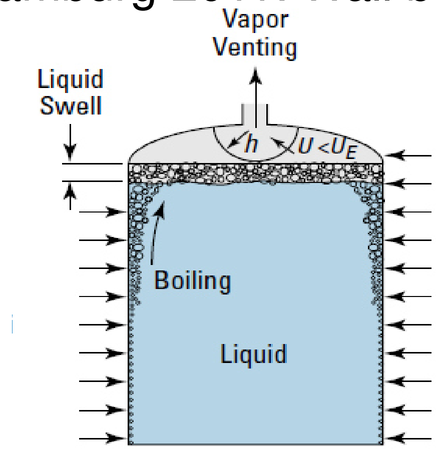
## Alternative models: vapor generation not uniform

FAI 1983-27: Non boiling region




- Because of the pressure head.
- Gas disengagement is more efficient.

Fauske 2000 /
Arkady Hamburg 2011: Wall boiling




- proposed for $H_2O_2$ decomposition.
- Gas disengagement is much more efficient: level swell of wall boiling = 10% of that of churn turbulent

**Were there any visual observations for these configurations?**

*Fai 83-27,A summary of Multiphase flow methods, 1983*
*H. K. Fauske, "Properly size vents for nonreactive and reactive chemicals," Chem. Eng. Prog., Feb. 2000.*

# Last part

Bubbly – Churn-turbulent transition criterion

Vapor generation: uniform in the bulk ?

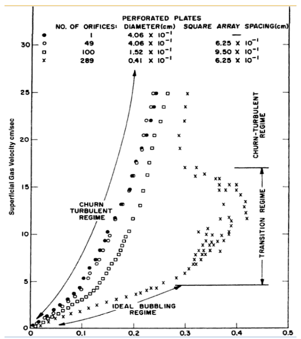
**Perspectives**

# Perspectives

- **Explore more recent experiments and correlations for reactor flow pattern.**

**From,**

Zuber & Hench (1962)




Zuber & Findlay $j_g = f(C_0)$ (1965)

**to**

Ishii 1977

Katoaka et al. 1987

Hibiki et al. 2003

Schlegel et al. 2010

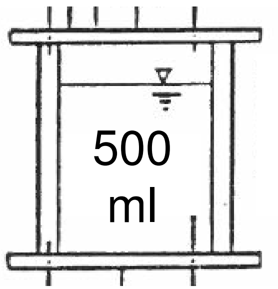
**An advice about the right correlation?**



MINES Saint-Étienne

# Perspectives

- **Make small scale visualization tests** (inspired by Wehmeier and Friedel)
  - **Condition:**
    - 500 ml jacketed reactor
    - Reaction: esterification




  - **Purposes:**
    - Observe bubble generation (initial size) and flow pattern during a runaway reaction
    - Observe sensitivity to different parameters
      - Concentration (solvent or excess of one reactant)
      - Reaction rate (catalysis)
      - Surface tension (surfactant)
      - Viscosity (thickening agent)
    - Compare with correlations developed for non reactive systems.

## Perspectives

**Extend approach to:**

- **Viscous system**
  - Addition of a thickening agent
  - Comparison with Acrylic Acid polymerization
- **Tempered hybrid system**
  - $H_2O_2$ decomposition

# Thank you for your attention!

www.mines-stetienne.fr

Une école de l'Institut Mines-Télécom

INSPIRING INNOVATION INNOVANTE PAR TRADITION

# Question list

- **Viscosity** linked to a special definition of bubbly flow ?
- Is **bubbly** flow a quite rare occurrence ?
- What about our **flow pattern determination proposal ?**
- Useful to model a **flow pattern changing system** ?
- Homogeneous = **foamy behavior** ?
- **Interfacial, often large bubble generation** ?
- Influence of **initial bubble size** on reactor flow pattern ?
- Interfacial bubble generation →**uniform vapor generation** ?
- Articles about runaway reaction **visualization**?
- **Visualization** during the large-scale DIERS experiments?
- Visualization for non uniform vapor generation?
- An advice about the **correlation** for flow pattern?