NETL 2013 Workshop on Multiphase Flow Science, Morgantown

Stability-Constrained Multi-Fluid CFD Models for Multiphase Systems

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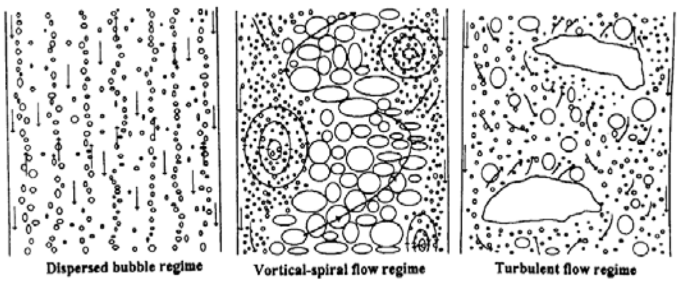
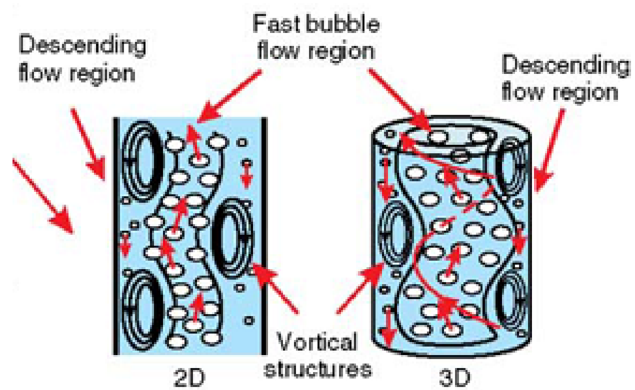
Complexity: *Multiscale structure formation and evolution*

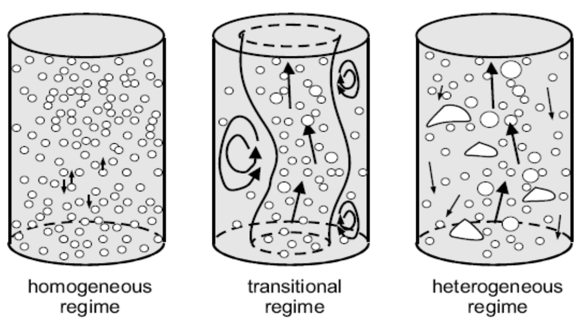
- **Macro-scale:** different flow regimes and regime transition
- **Meso/Micro-scales:** liquid vortices, bubble wakes, bubble swarms, bubble deformation, bubble breakup/coalescence



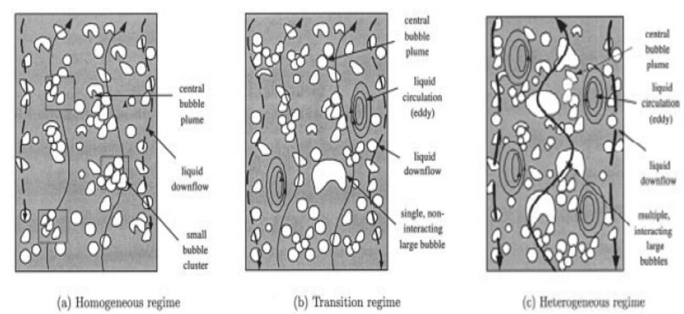
Chen et al., AIChE J., 1994



Lin et al., AIChE J., 1996



Harteveld., 2005



Ruthiya et al., AIChE J., 2005

State of The Art: CFD simulation

- Model-dominated
- Force models: drag, virtual mass, lift, turbulent dispersion force, etc.
- Turbulence models: different choice for single-phase turbulence, bubble-induced turbulence, dispersed or mixture model for two-phase turbulence, turbulence coupling
- Discretization schemes for convection term
- Grid resolution
- Boundary condition
- fails to work for higher gas flow rate (Transition & heterogeneous regime)
- NOT able to predict the regime transition

See Monahan et al., AIChE J., 2005

Requirements: CFD simulation

- Capture the dominant structures among the multi-scales

  not only the macro-scale phase distribution

- Cover all the regimes

  not only a single specific regime

- Predict the structure evolution (regime transition)

  not only the evolution within each regime

Challenging problems

Macro-scale: *regime transition, why？*

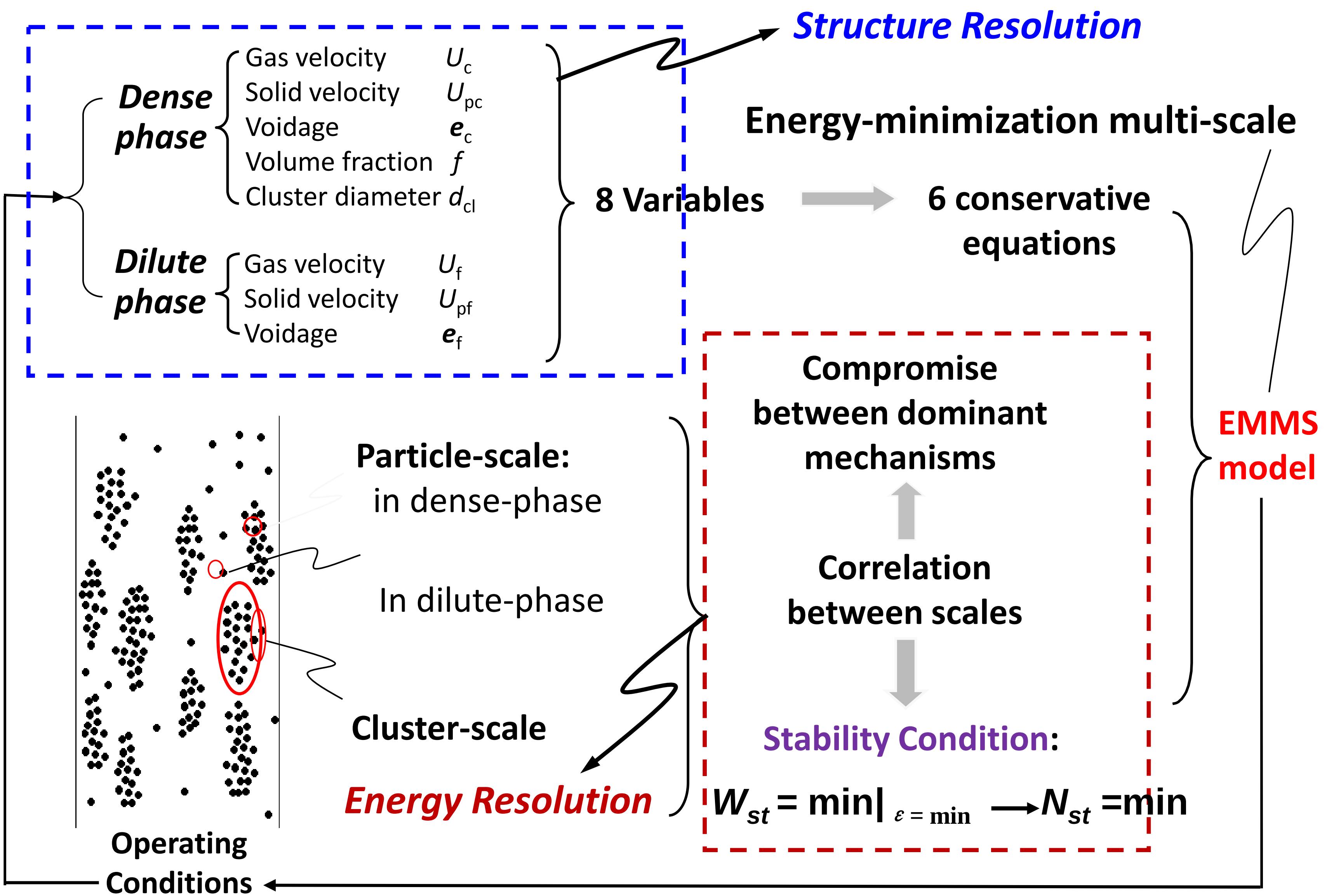
?

Meso/Micro-scales: *how to describe the gas-liquid interaction？*

?

How can we incorporate the meso/micro effects into CFD simulation without the need to reconstruct the missing structure using DNS?

The EMMS model: Originally proposed for gas-solid fluidization



(*Li & Kwauk, 1989*)

The hierarchy in the EMMS model

(1): Mass and force balances

Force balance equation for the dense phase

$$\frac{3}{4}C_{\mathrm{Dc}}\frac{\rho_{\mathrm{g}}U_{\mathrm{sc}}^{2}}{d_{\mathrm{p}}}=\frac{1-\varepsilon}{1-\varepsilon_{\mathrm{c}}}\left(\rho_{\mathrm{p}}-\rho_{\mathrm{g}}\right)g$$

Force balance equation for the dilute phase

$$\frac{3}{4}C_{\mathrm{Df}}\frac{\rho_{\mathrm{g}}U_{\mathrm{sf}}^{2}}{d_{\mathrm{p}}}=\left(\rho_{\mathrm{p}}-\rho_{\mathrm{g}}\right)g$$

Force balance of interphase

$$\frac{3}{4}C_{\mathrm{Di}}\frac{\rho_{\mathrm{g}}U_{\mathrm{si}}^{2}}{d_{\mathrm{cl}}}=\left(\varepsilon-\varepsilon_{\mathrm{c}}\right)\left(\rho_{\mathrm{p}}-\rho_{\mathrm{g}}\right)g$$

Continuity of solid

$$U_{\mathrm{p}}=fU_{\mathrm{pc}}+(1-f)U_{\mathrm{pf}}$$

Continuity of fluid

$$U_{\mathrm{g}}=fU_{\mathrm{c}}+(1-f)U_{\mathrm{f}}$$

(2): Correlation of meso-scale structure and meso-scale energy dissipation

Cluster diameter

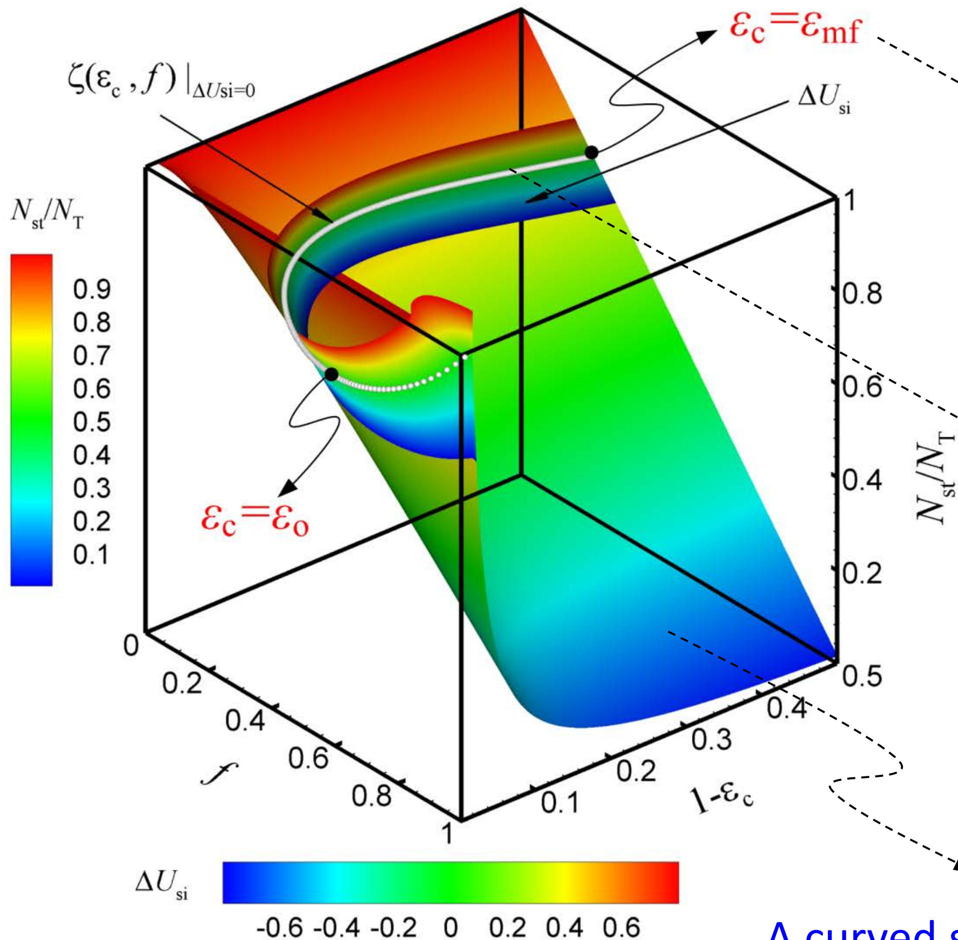
$$d_{\mathrm{cl}}=\frac{\left(\rho_{\mathrm{p}}-\rho_{\mathrm{g}}\right)gU_{\mathrm{p}}/\rho_{\mathrm{p}}(1-\varepsilon_{\max})-N_{\mathrm{st,mf}}}{N_{\mathrm{st}}-N_{\mathrm{st,mf}}}d_{\mathrm{p}}$$

(3): Stability condition

$$N_{\mathrm{st}}=\left[U_{\mathrm{g}}-\frac{\varepsilon_{\mathrm{f}}-\varepsilon}{1-\varepsilon}f(1-f)U_{\mathrm{f}}\right]\frac{\left(\rho_{\mathrm{p}}-\rho_{\mathrm{g}}\right)g}{\rho_{\mathrm{p}}}=\min$$

Yang, Progress in CFD, 2012; Chen et al., Chinese J Chem. Eng., 2012

Regime transition (choking)： The role of different constraints



Two points： final solution subject to the stability condition

A curve： due to the correlation of meso-scale structure and meso-scale energy dissipation

A curved surface： solutions of mass and force balances

System complexity

Yang, Progress in CFD, 2012; Chen et al., Chinese J Chem. Eng., 2012

Gas-Solid: Application of EMMS drag in CFD simulation of a CFB riser

Two-Fluid Model

(Wen-Yu/Ergun drag laws)

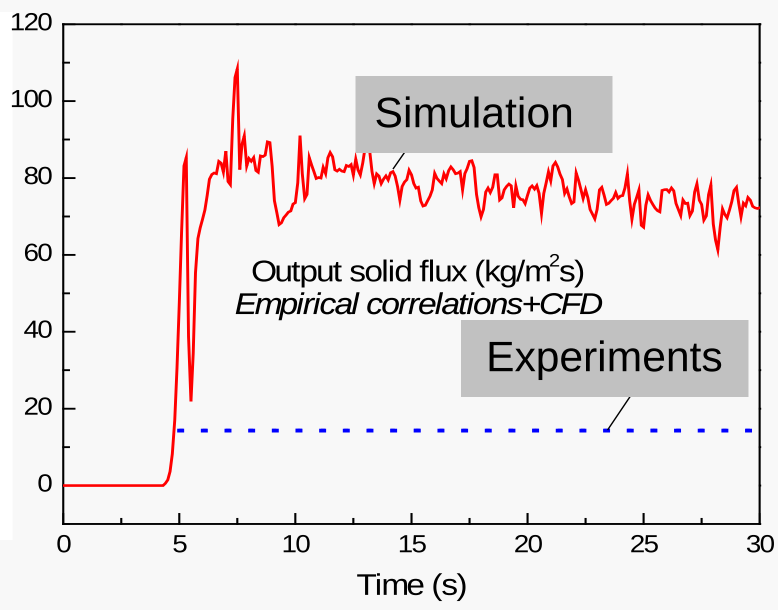
Two-Fluid Model

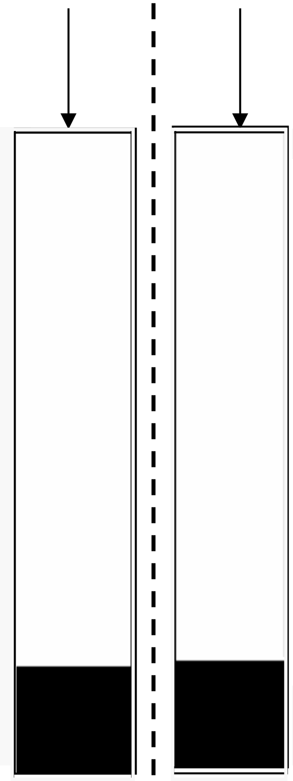
(EMMS drag model)

Homogeneous

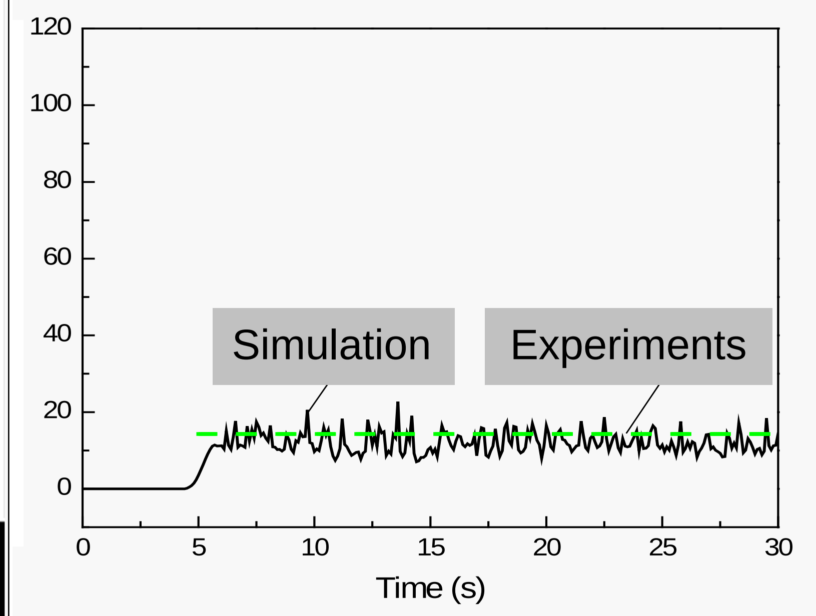
Clusters

Output particle flux





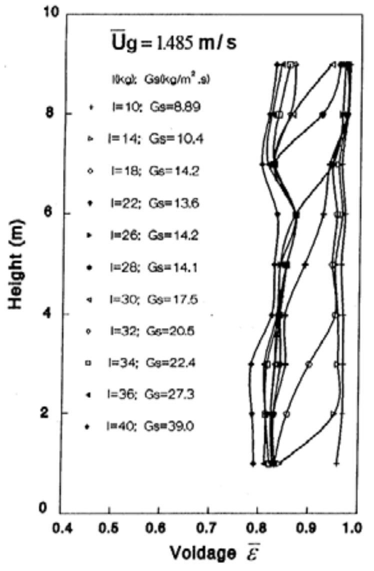
Output particle flux



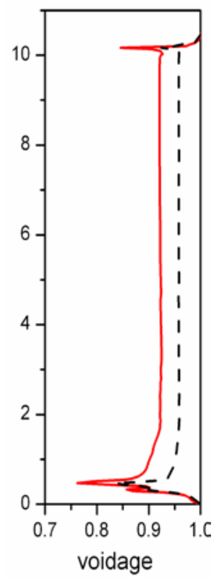
Yang et al., Ind. Eng. Chem. Res., 2004, 43, 5548-5561. Yang et al., Chem. Eng. J,, 2003

Axial distribution of solid concentration in a CFB riser

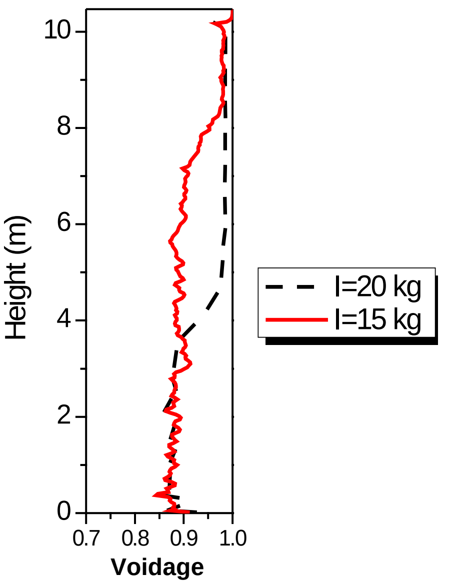
Experiment:
Dense bottom, dilute top



Two Fluid Model (TFM)
Homogeneous



TFM+EMMS
Dense bottom, dilute top



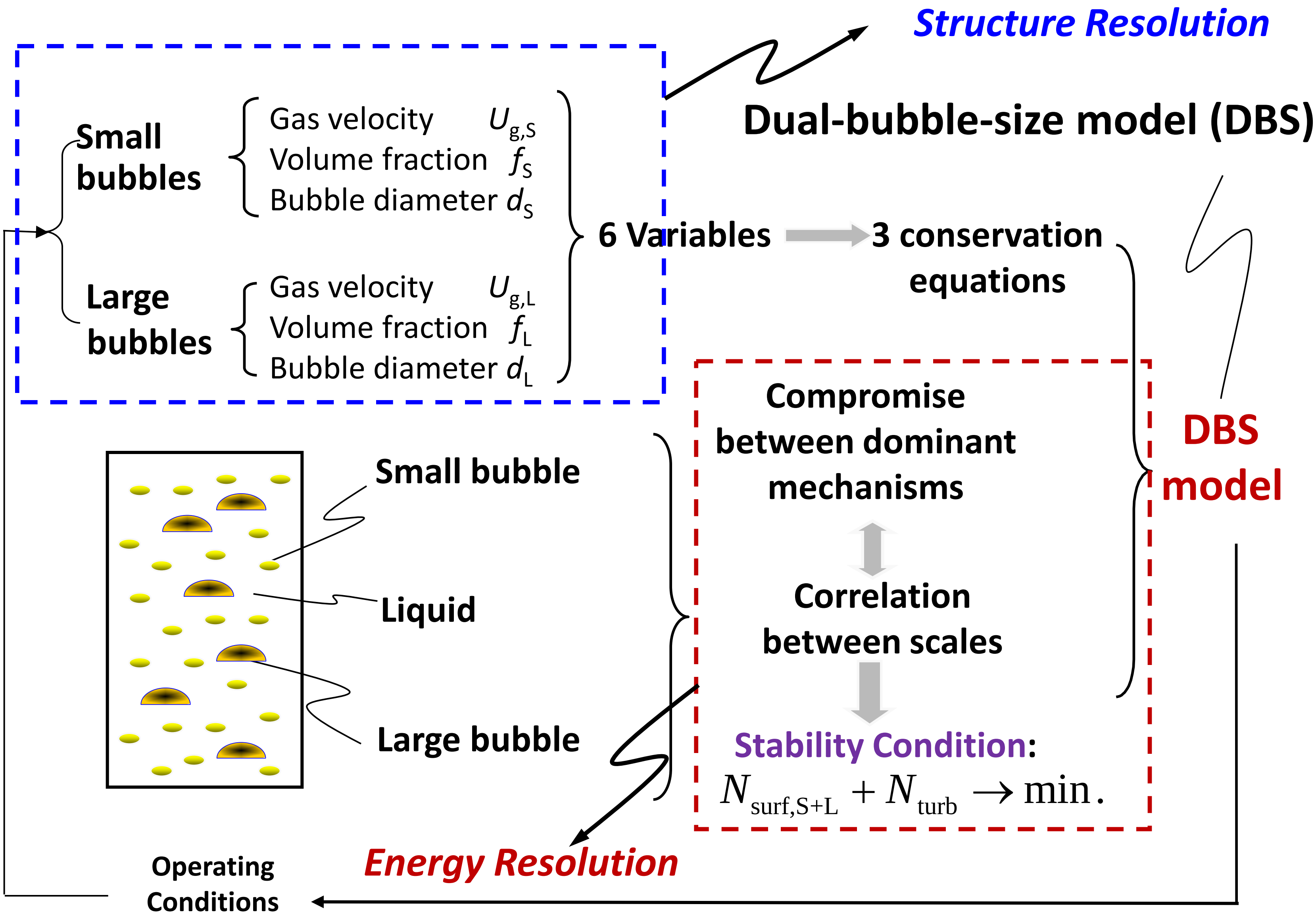
U_g=1.52m/s, G_s=14.3Kg/m^2s

The system can be self-adapted due to cluster formation!

Weinstein et al., Fluidization IV, 1983, 299-306;
Li et al., Chem. Eng. Sci., 1998, 3367-3379

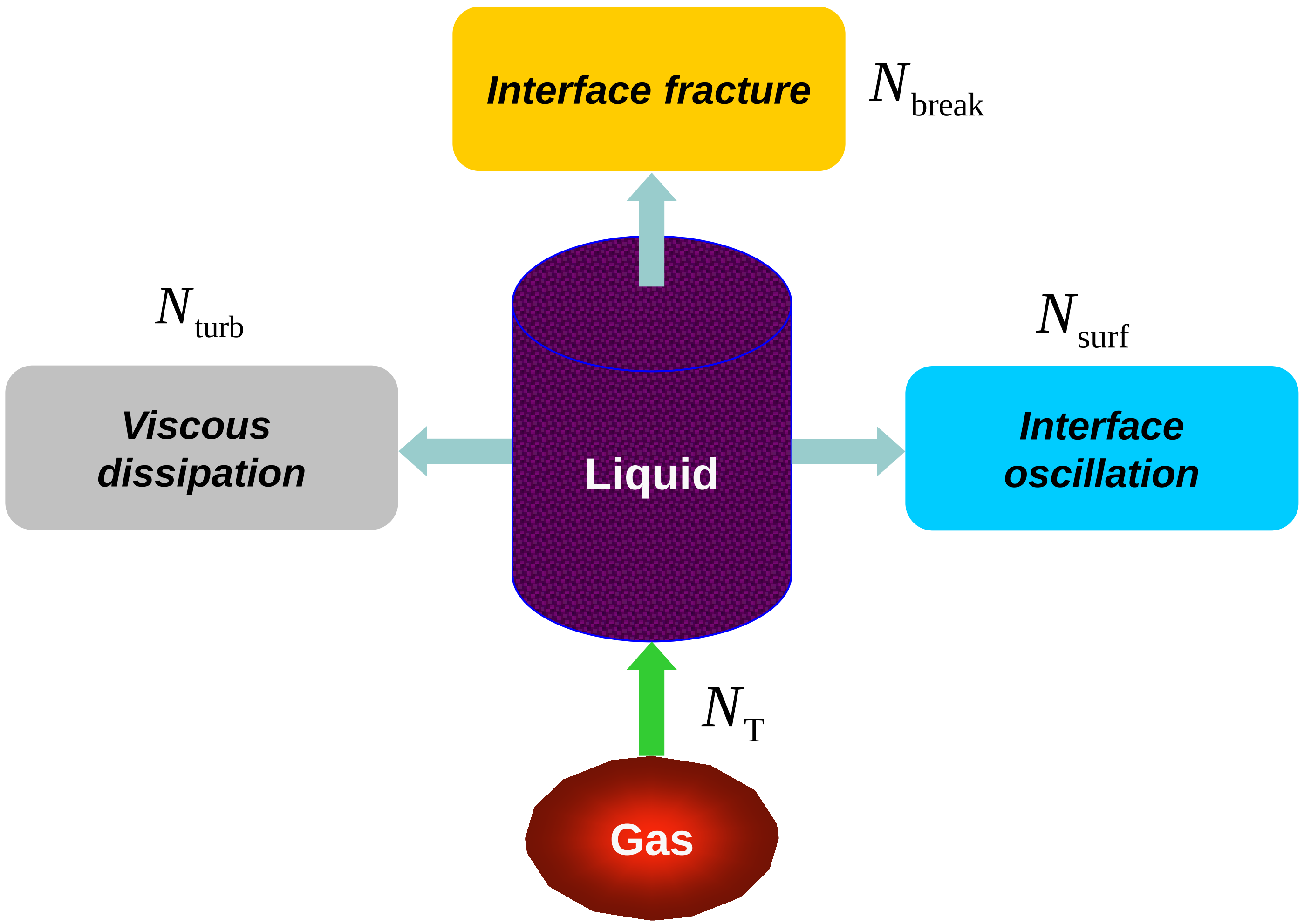
Yang et al., Ind. Eng. Chem. Res., 2004, 43, 5548-5561;
Yang et al., CFB VIII, 2005, 291-298.

Extension to Gas-liquid system

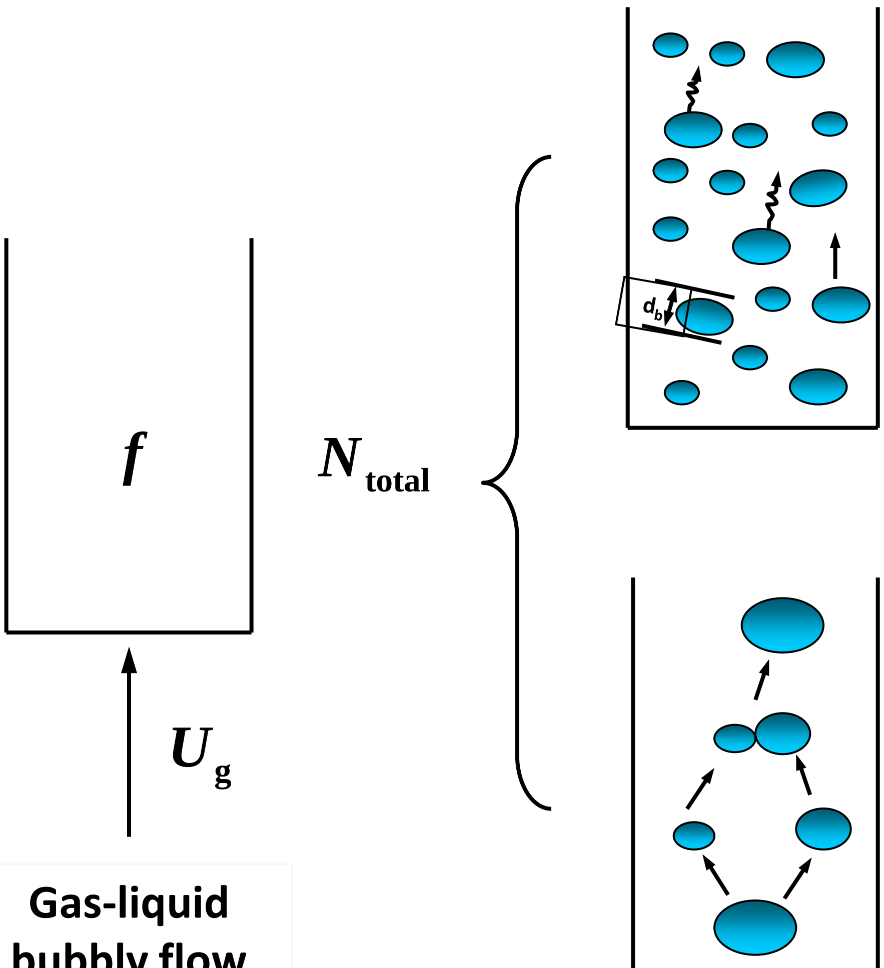


(*Yang et al, Chem. Eng. Sci, 2007*)

Path of energy transfer and dissipation *(Zhao, 2006; Ge et al, CES,2007)*



Scale-dependent energy resolution



Gas-liquid bubbly flow

Energy dissipated directly on *micro-scale* caused by relative motion between bubbles and liquid

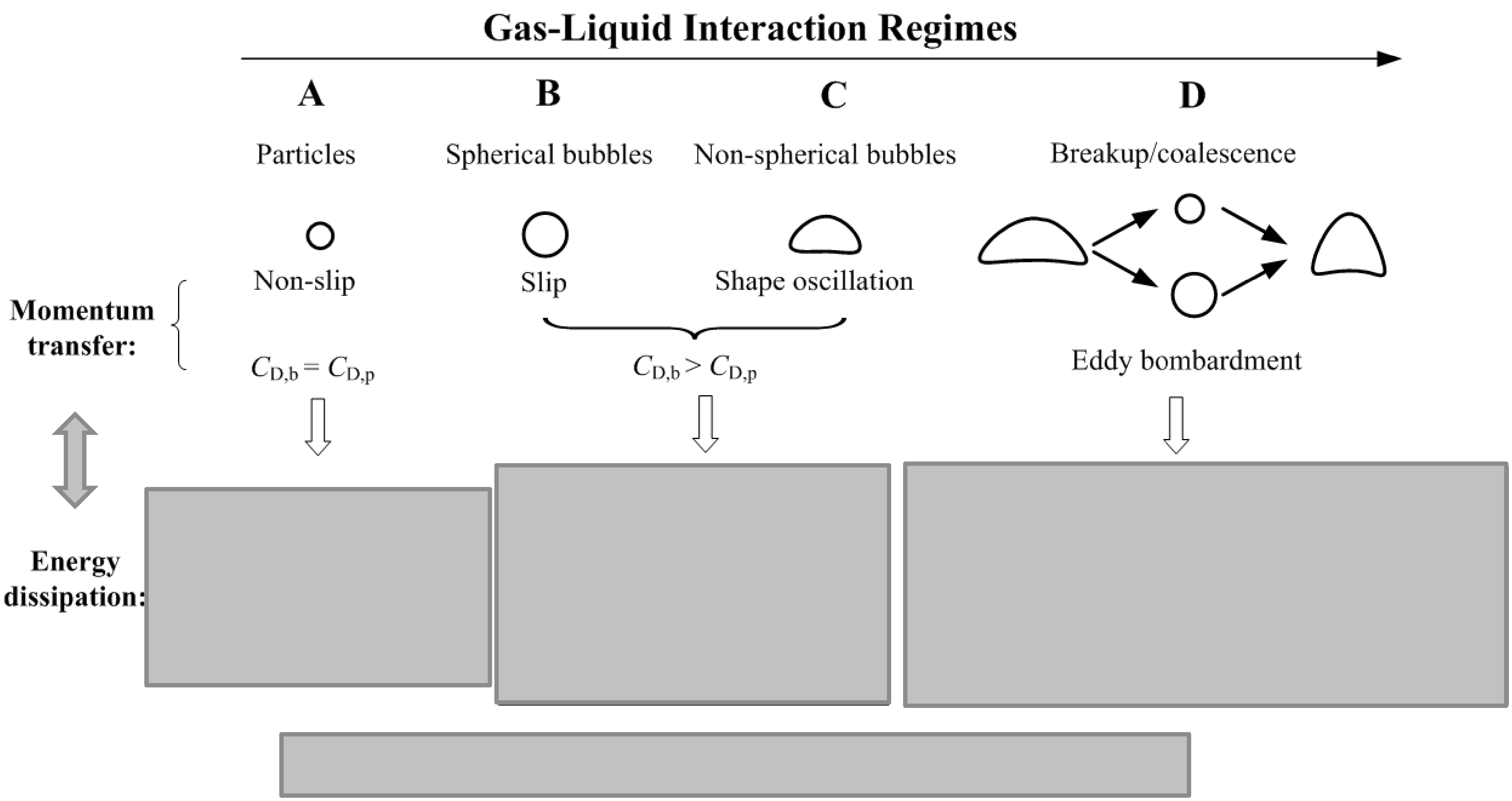
$$N_{surf} + N_{turb} \longrightarrow \textbf{min}$$

Energy consumption due to *meso-scale* structure evolution

$$N_{break} \longrightarrow \textbf{max}$$

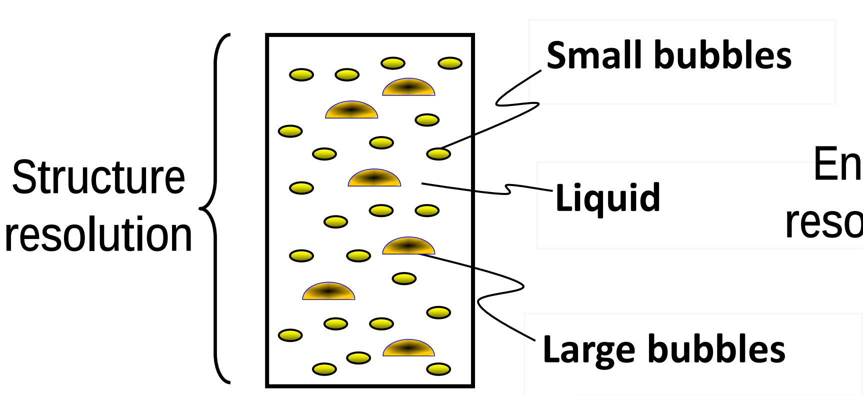
(Zhao, PhD thesis, 2006; Ge et al, Chem. Eng. Sci.,2007)

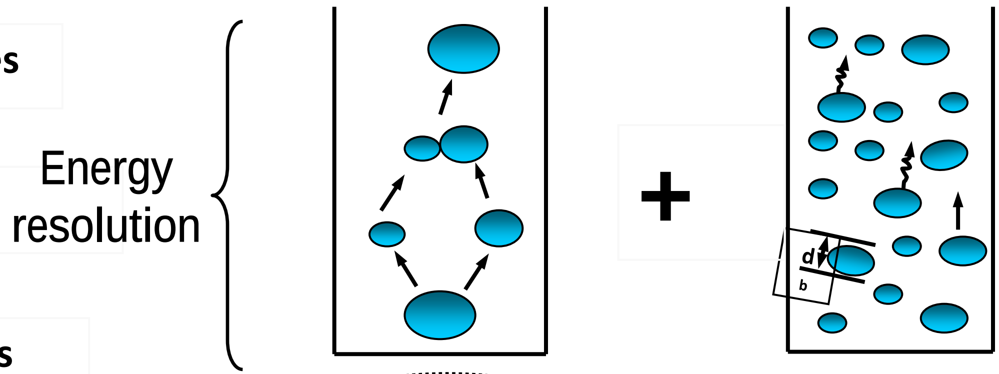
Relationship of momentum transfer and energy dissipation



(*Yang et al, Chem. Eng. Sci., 2010, 2011*)

A new mechanism beyond transport equations





A buffer for energy dissipation ⇒

Meso-scale dissipation

Sustain the formation and evolution of mesoscale structure

$N_{break} \longrightarrow$ **max**

Micro-scale dissipation

dissipated directly by relative motion of bubbles and liquid

$N_{surf} + N_{turb} \longrightarrow$ **min**

Stability condition

⇐

Transport equations:

Mass and momentum conservative equations (6 structure parameters), not closed!

Model assumption

- (viscous dissipation) $N_{turb} \approx \varepsilon$ (turbulent dissipation)
- $N_{break} \rightleftharpoons N_{coalescence}$ (No net surface generated)
- Classical statistical theory of isotropic turbulence

(Luo & Svendsen, AIChE J., 1996)

$$N_{\mathrm{break}} = \int_{\lambda_{\min}}^{d_{\mathrm{b}}} \int_{0}^{0.5} \frac{\omega(d_{\mathrm{b}}, \lambda)}{(1-f_{\mathrm{b}})\rho_{\mathrm{l}} + f_{\mathrm{b}}\rho_{\mathrm{g}}} \cdot P_{\mathrm{b}}(d_{\mathrm{b}}, \lambda, f_{\mathrm{BV}}) \cdot c_{\mathrm{f}} \pi d_{\mathrm{b}}^{2} \sigma \cdot \mathrm{d}f_{\mathrm{BV}} \mathrm{d}\lambda = \varphi(\varepsilon, f_{\mathrm{b}}, d_{\mathrm{b}})$$

- $$N_{\mathrm{surf}} = \left[1 - \frac{C_{\mathrm{D,p}}}{C_{\mathrm{D,b}}}\right] N_{\mathrm{T}}$$

Mathematical model (DBS):

Variables: $(f_S, f_L, d_S, d_L, U_{gS}, U_{gL})$ ⟹ the 6D space of structure parameter

Equations:

Small bubble:

$$f_S \rho_l g = \frac{f_S}{\pi/6 \cdot d_S^3} \cdot C_{DS} \frac{\pi}{4} d_S^2 \cdot \frac{1}{2} \rho_l \left(\frac{U_{g,S}}{f_S} - \frac{U_l}{1-f_b} \right)^2$$

Large bubble:

$$f_L \rho_l g = \frac{f_L}{\pi/6 \cdot d_L^3} \cdot C_{DL} \frac{\pi}{4} d_L^2 \cdot \frac{1}{2} \rho_l \left(\frac{U_{g,L}}{f_L} - \frac{U_l}{1-f_b} \right)^2$$

Continuity:

$$U_{g,S} + U_{g,L} = U_g$$

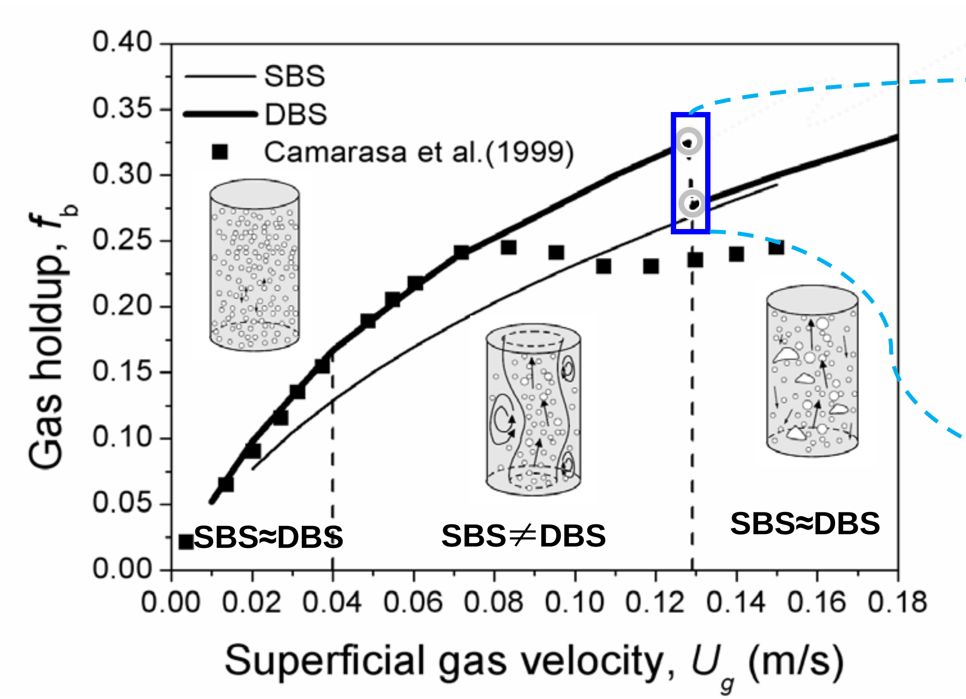
subject to → **Stability condition:**

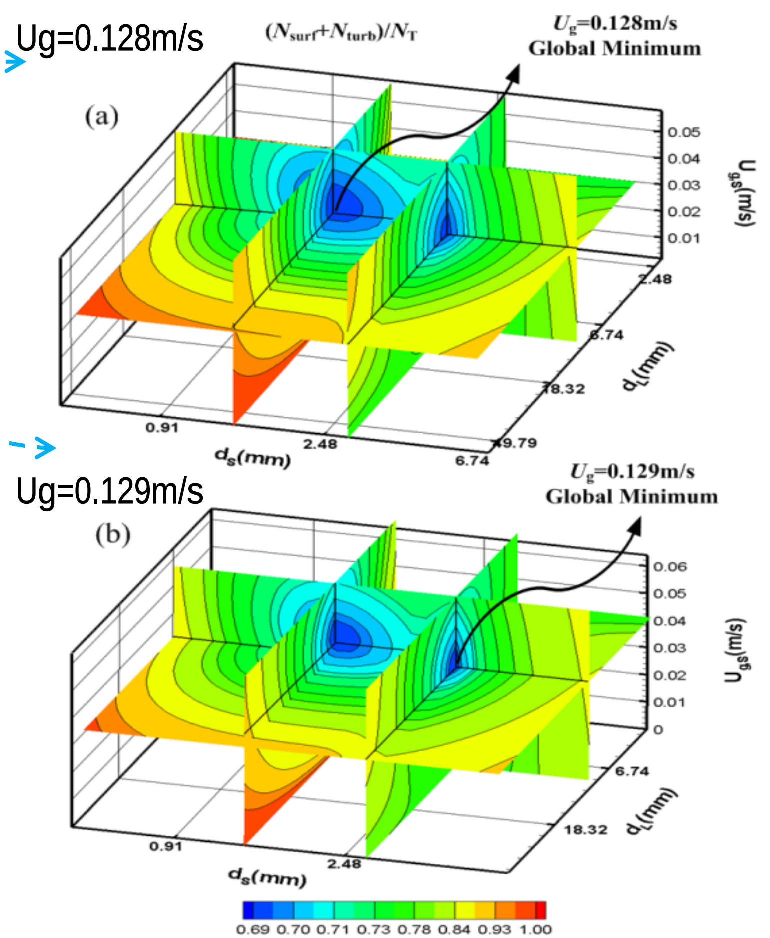
$$N_{surf,S+L} + N_{turb} \rightarrow \min.$$

Regime transition: why?

Jump change of global minimum of micro-scale energy dissipation within the space of structure parameters

Jump change of total gas hold-up





Camarasa et al., 1999, Chem. Eng. Proc., 38, 329-344;
Ruthiya et al., 2005, AIChE Journal, 1951-1965

Yang, et al., Chem. Eng. Sci., 2010, 65, 517-526;
Chen, et al., IECR, 2009, 48, 290-301

Stability-constrained multi-fluid approach (SCMF)

DBS Model:

- Mass balance
- Force balance
- Closure (stability condition)

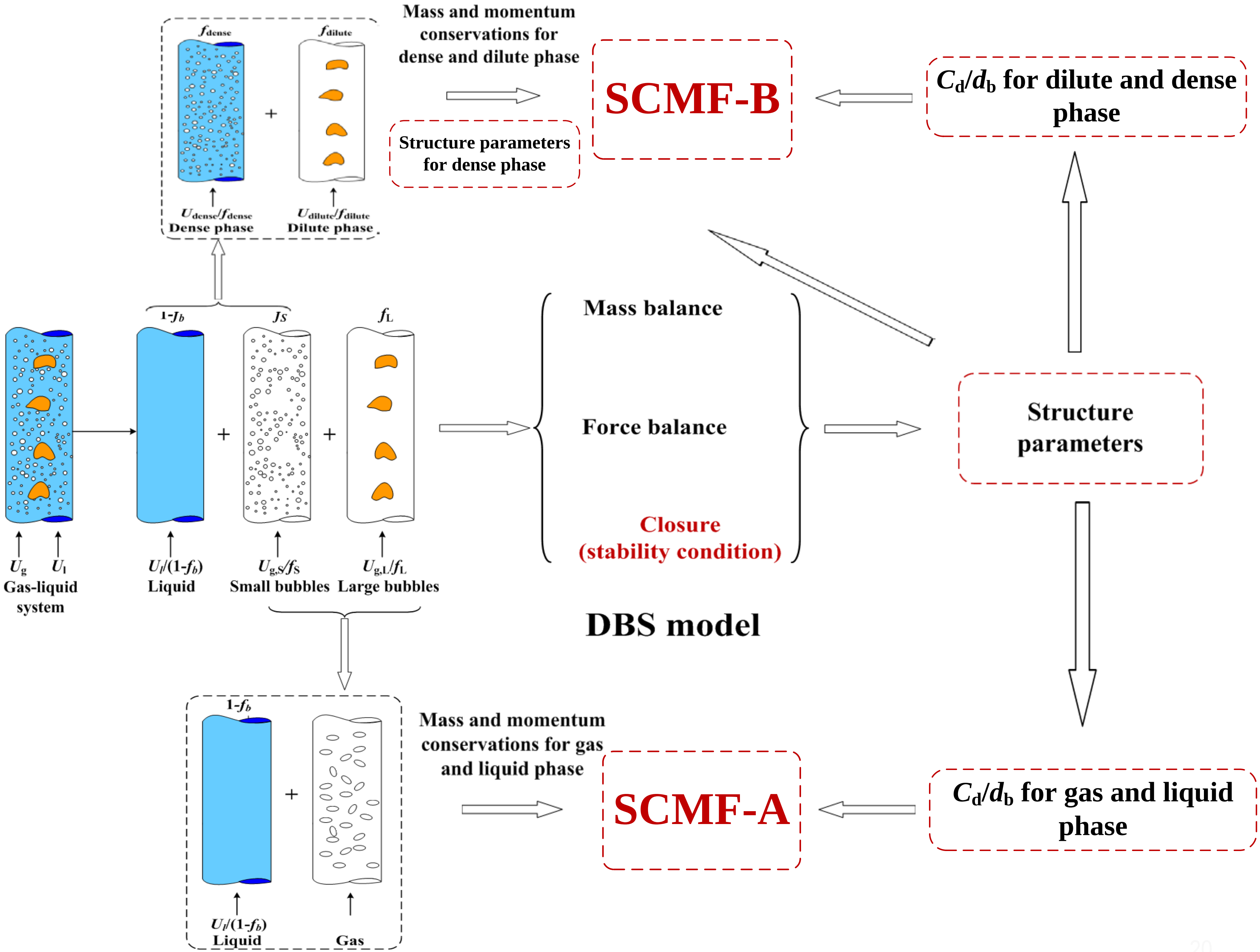
vs.

Two-fluid models:

- Mass conservation
- Momentum conservation
- Closure (Empirical)

Stability-constrained multi-fluid approach (SCMF)

- Mass conservation for two or multiple fluids
- Momentum conservation for two or multiple fluids
- **Closure (stability condition)**



f_{dense}
f_{dilute}
U_{dense}/f_{dense}
Dense phase
U_{dilute}/f_{dilute}
Dilute phase
Mass and momentum conservations for dense and dilute phase
Structure parameters for dense phase
SCMF-B
C_d/d_b for dilute and dense phase
$1-f_b$
f_S
f_L
U_g
U_l
Gas-liquid system
$U_l/(1-f_b)$
Liquid
$U_{g,S}/f_S$
Small bubbles
$U_{g,L}/f_L$
Large bubbles
Mass balance
Force balance
Closure (stability condition)
Structure parameters
DBS model
$1-f_b$
$U_l/(1-f_b)$
Liquid
Gas
Mass and momentum conservations for gas and liquid phase
SCMF-A
C_d/d_b for gas and liquid phase

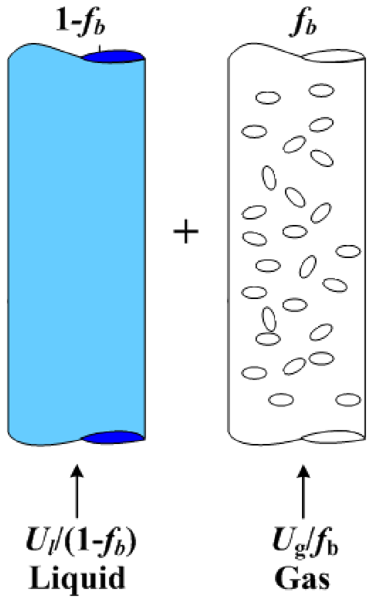
SCMF-A

Mass conservations:

$$\frac{\partial(\varepsilon_l \rho_l)}{\partial t} + \nabla\cdot(\varepsilon_l \rho_l \vec{u}_l) = \Gamma_{liquid\_S} + \Gamma_{liquid\_L} = \Gamma_{liquid\_gas} \quad (1)$$

(2)+(3):

$$\frac{\partial(\varepsilon_g \rho_g)}{\partial t} + \nabla\cdot(\varepsilon_g \rho_g \vec{u}_g) = \Gamma_{L\_liquid} + \Gamma_{S\_liquid} = \Gamma_{gas\_liquid}$$



Assumption:

$$\vec{u}_S = \vec{u}_L = \vec{u}_g$$

Momentum conservations:

$$\frac{\partial(\varepsilon_l \rho_l \vec{u}_l)}{\partial t} + \nabla\cdot(\varepsilon_l \rho_l \vec{u}_l \vec{u}_l) = -\varepsilon_l \nabla P + \mu_{l,eff}\,\varepsilon_l\left[\nabla\vec{u}_l + (\nabla\vec{u}_l)^T\right] + \varepsilon_l \rho_l g + \boldsymbol{M}_{liquid\_gas} \quad (4)$$

(5)+(6):

$$\frac{\partial(\varepsilon_g \rho_g \vec{u}_g)}{\partial t} + \nabla\cdot(\varepsilon_g \rho_g \vec{u}_g \vec{u}_g) = -\varepsilon_g \nabla P + \mu_{g,eff}\,\varepsilon_g\left[\nabla\vec{u}_g + (\nabla\vec{u}_g)^T\right] + \varepsilon_g \rho_g g + \boldsymbol{M}_{gas\_liquid}$$

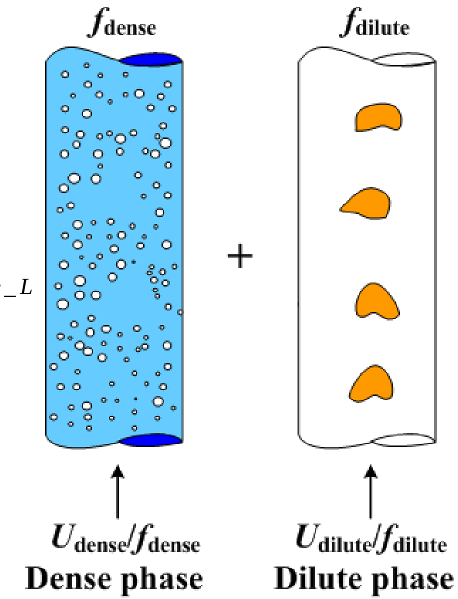
SCMF-B

Mass conservations:

(1)+(2):

$$\frac{\partial(\varepsilon_{dense}\rho_{dense})}{\partial t}+\nabla\cdot(\varepsilon_{dense}\rho_{dense}\vec{u}_{dense})=\Gamma_{liquid\_L}+\Gamma_{S\_L}=\Gamma_{dense\_L}$$

$$\frac{\partial(\varepsilon_L\rho_L)}{\partial t}+\nabla\cdot(\varepsilon_L\rho_L\vec{u}_L)=\Gamma_{L\_liquid}+\Gamma_{L\_S}=\Gamma_{L\_dense} \qquad (3)$$



Assumption:

$$\vec{u}_S=\vec{u}_l=\vec{u}_{dense}$$

$$\boldsymbol{M}_{S\_L}=\boldsymbol{M}_{L\_S}=0$$

$$\varepsilon_{dense}=\varepsilon_l+\varepsilon_S$$

$$\rho_{dense}=\frac{\varepsilon_l}{\varepsilon_l+\varepsilon_S}\rho_l+\frac{\varepsilon_S}{\varepsilon_l+\varepsilon_S}\rho_S$$

Momentum conservations:

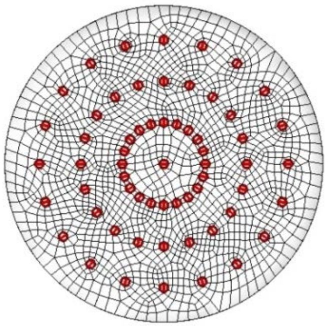
(4)+(5):

$$\frac{\partial(\varepsilon_{dense}\rho_{dense}\vec{u}_{dense})}{\partial t}+\nabla\cdot(\varepsilon_{dense}\rho_{dense}\vec{u}_{dense}\vec{u}_{dense})=-(\varepsilon_{dense})\nabla P$$
$$+\left\{(\mu_{l,eff}\varepsilon_l+\mu_{S,eff}\varepsilon_S)\left[\nabla\vec{u}_S+(\nabla\vec{u}_S)^T\right]\right\}+(\varepsilon_{dense}\rho_{dense})g+\boldsymbol{M}_{dense\_L}$$

$$\frac{\partial(\varepsilon_L\rho_L\vec{u}_L)}{\partial t}+\nabla\cdot(\varepsilon_L\rho_L\vec{u}_L\vec{u}_L)=-f_L\nabla P+\mu_{L,eff}\varepsilon_L\left[\nabla\vec{u}_L+(\nabla\vec{u}_L)^T\right]+\varepsilon_L\rho_L g+\boldsymbol{M}_{L\_dense} \qquad (6)$$

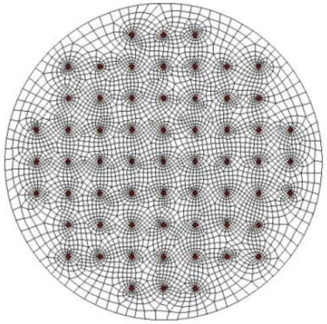
Simulation case:
Hills (1974)

- Height: 1.3m; ID: 0.138m
- Initial liquid height: 0.9 m
- Perforated plate: 61 holes
- hole diameter: 2mm(0.4mm)
- Number of meshes: 5.31 million
- k-ε mixture model
- First order upwind
- Time averaged data for H=0.6m



Simulation case:
Camarasa et al. (1999)

- Height: 2m; ID: 0.1m
- Initial liquid height: 1.35 m
- Perforated plate: 61 holes
- hole diameter: 1mm
- Number of meshes: 3.34 million
- k-ε mixture model
- First order upwind
- Time averaged data for H=1m



SCMF-A vs. other drag models (C_{d0}, p, d_b)

Effective drag coefficient: $C_D = C_{D0}(1-\varepsilon_g)^p$

Correlations

Standard drag coefficient

$$C_{D0} = \max\{\min[\frac{16}{Re}(1+0.15\,Re^{0.687}), \frac{48}{Re}], \frac{8}{3}\frac{Eo}{Eo+4}\}$$

Tomiyama (1998)

$$C_{D0} = 0.44 + \frac{24}{Re} + \frac{6}{1+\sqrt{Re}}$$

White (1974)

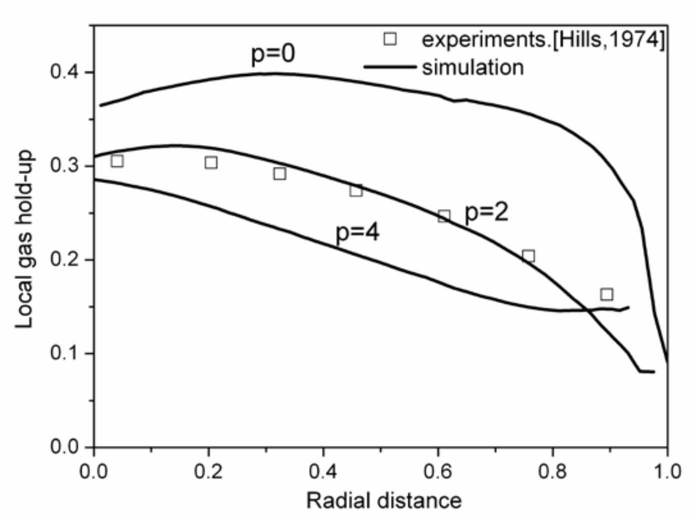
SCMF-A

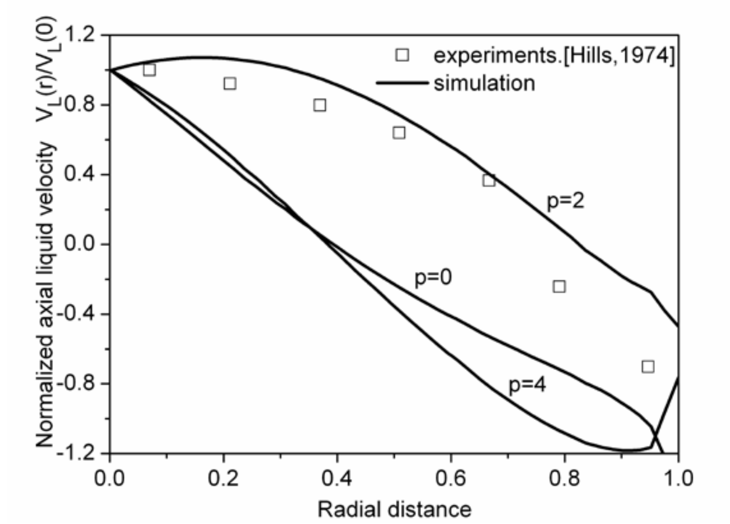
$$C_D / d_b = \begin{cases} 422.5 - 5335U_g + 21640.5U_g^2, & U_g \le 0.128 \\ 139.3 - 795U_g + 1500.3U_g^2, & U_g > 0.128 \end{cases}$$

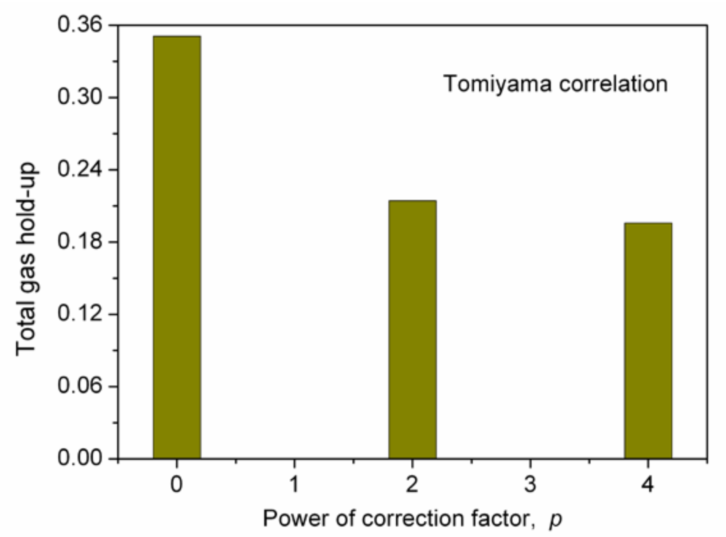
DBS model (this work)

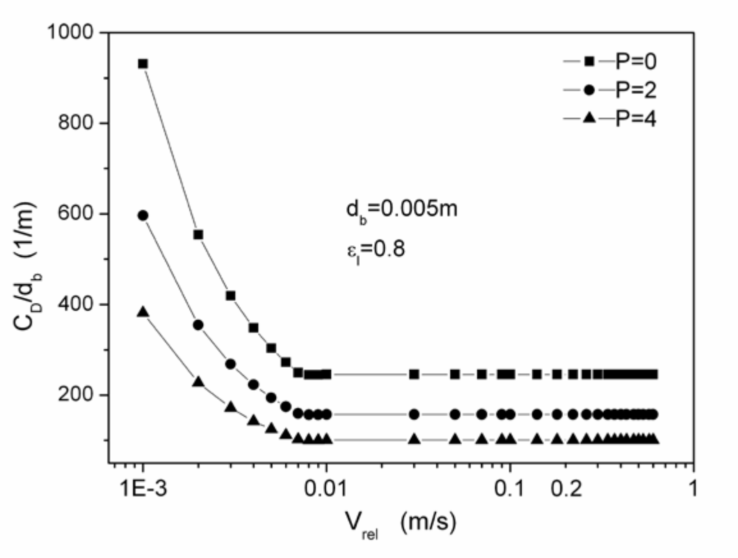
Effect of correction factor on simulation C_{D0}: Tomiyama; db=5mm; p: 0, 2, 4

$$C_D = C_{D0}(1-\varepsilon_g)^p$$





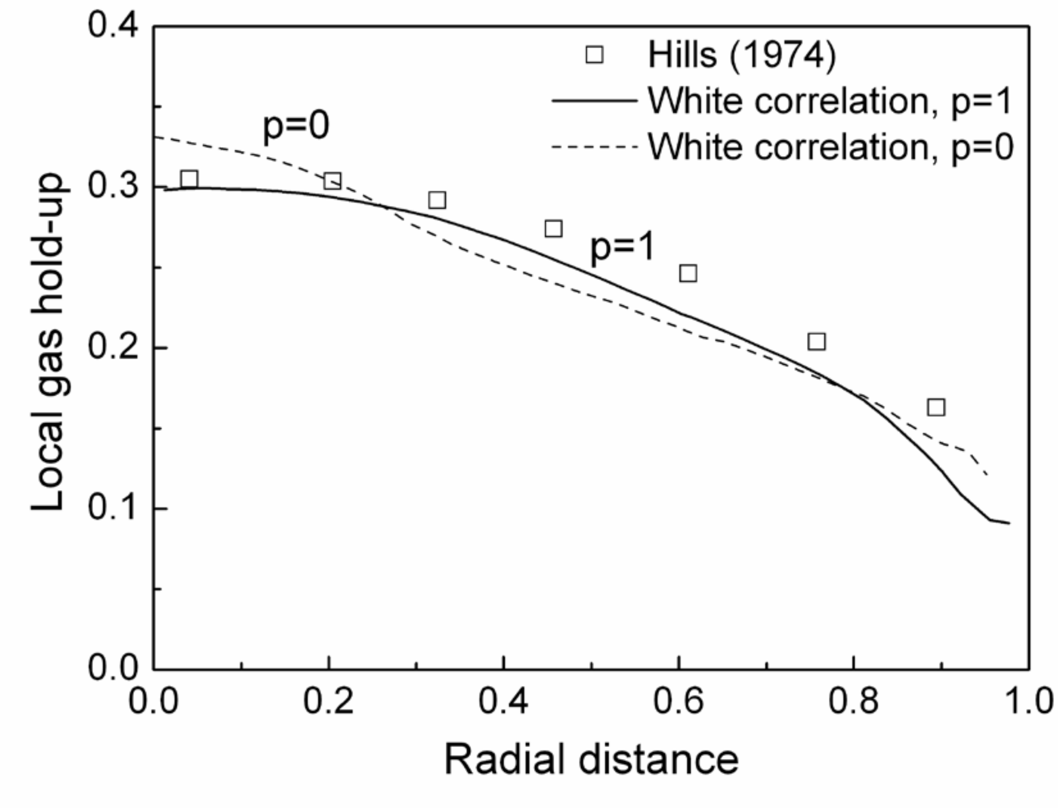




Ug=0.095m/s

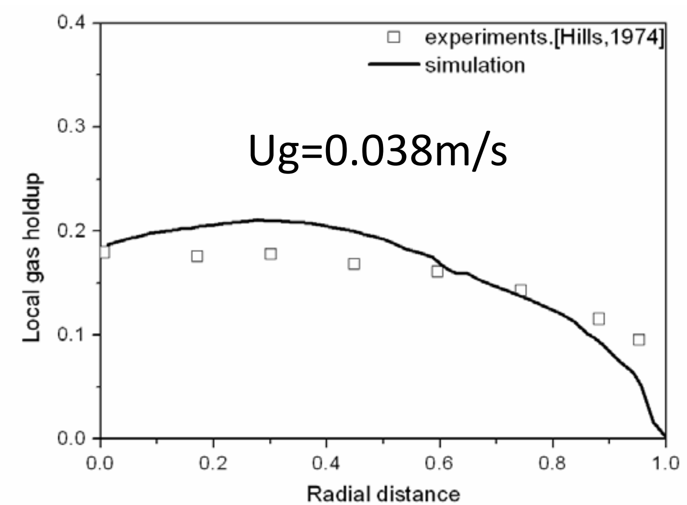
Effect of correction factor on simulation *C_{D0}: White; db=5mm; p: 0, 2, 4*

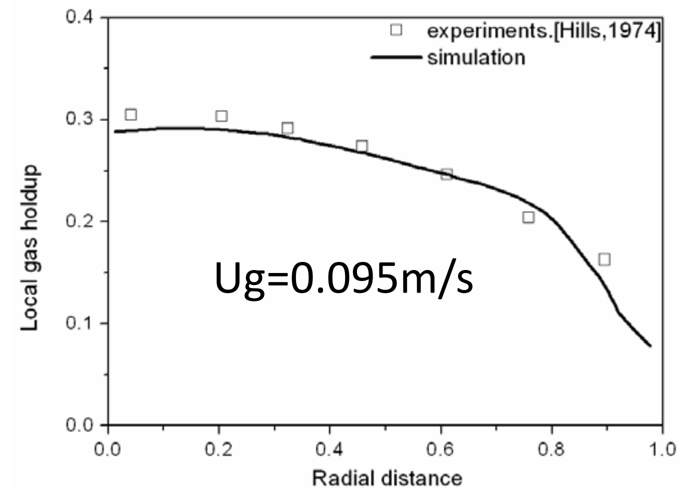
$$C_D = C_{D0}(1-\varepsilon_g)^p$$

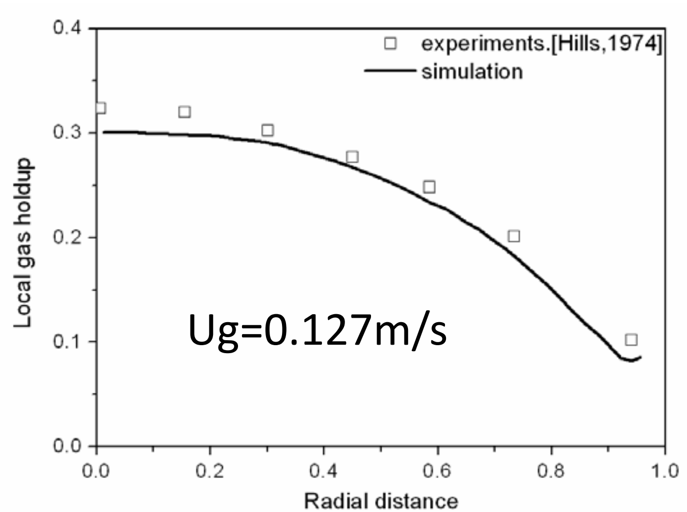


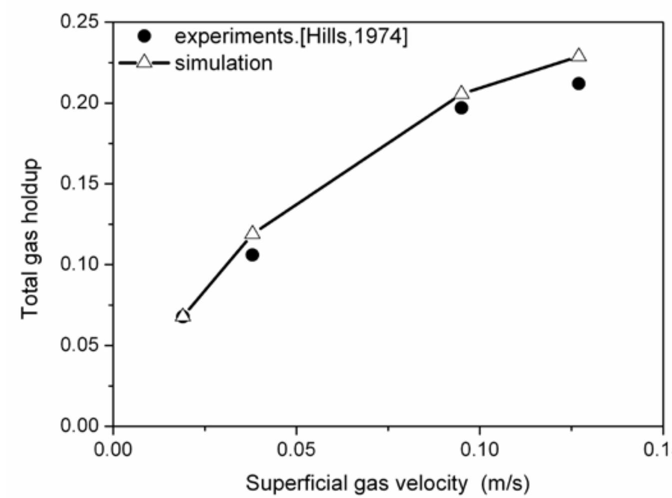
Ug=0.095m/s

Simulation with the SCMF-A model (Gas holdup)

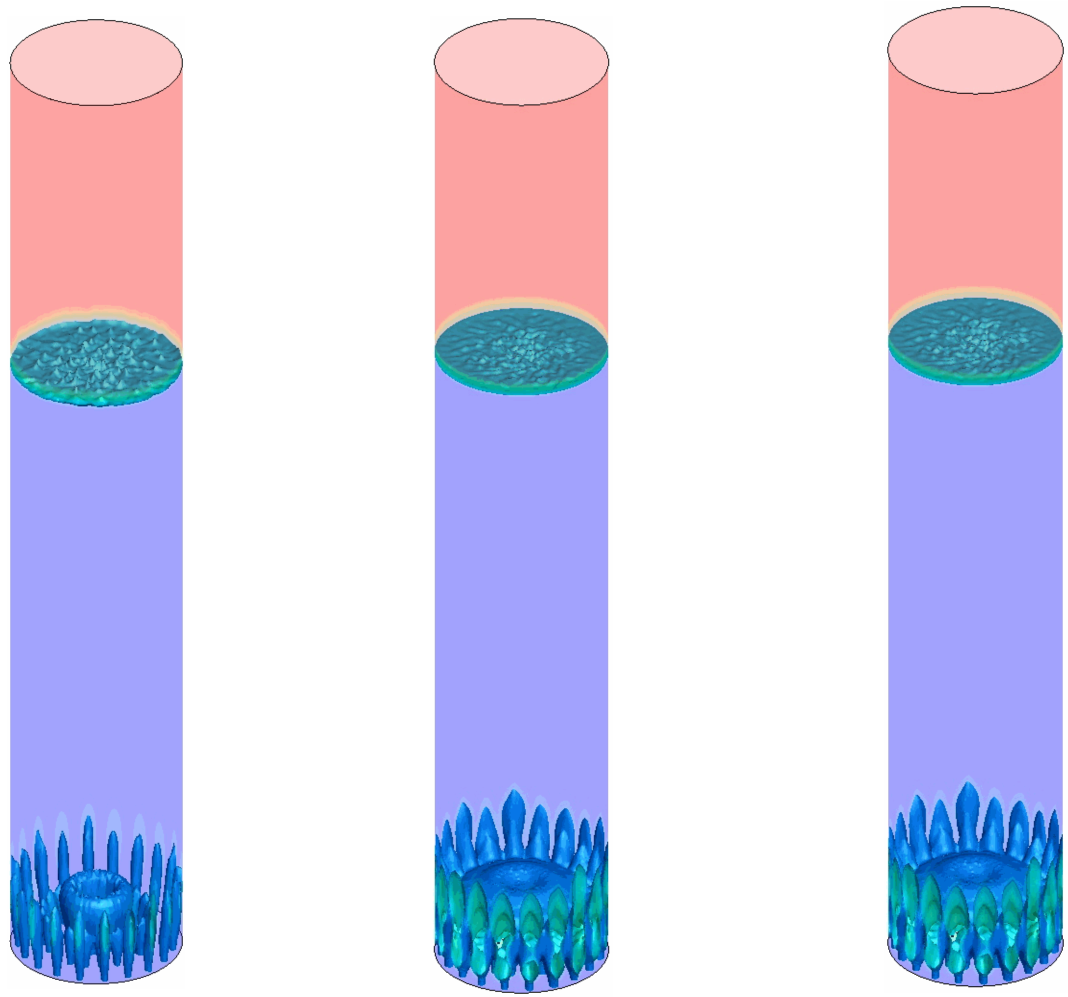








Simulation with the SCMF-A model



Ug=0.038m/s Ug=0.095m/s Ug=0.127m/s

SCMF-B vs. other drag models:

Schiller-Naumann

$$C_{D0} = \begin{cases} \frac{24}{\mathrm{Re}}\left(1+0.15\,\mathrm{Re}^{0.687}\right) & \mathrm{Re} \le 1000 \\ 0.44 & \mathrm{Re}>1000 \end{cases}$$

$$C_{\mathrm{D}} = C_{\mathrm{D0}}(1-\varepsilon_g)^p \qquad p=0$$

Ishii-Zuber

$$C_D = \begin{cases} \frac{24}{\mathrm{Re}}\left(1+0.1\mathrm{Re}^{0.75}\right), & \text{viscous regime} \\ \frac{2}{3} d_b \sqrt{\frac{g\Delta\rho}{\sigma}} \left\{ \frac{1+17.67\left[f\left(\varepsilon_g\right)\right]^{6/7}}{18.67 f\left(\varepsilon_g\right)} \right\}^2, & \text{distorted regime} \\ \frac{8}{3}\left(1-\varepsilon_g\right)^2, & \text{churn turbulent flow regime} \end{cases}$$

$$C_{\mathrm{D}} = C_{\mathrm{D0}}(1-\varepsilon_g)^p \qquad f\left(\varepsilon_g\right) = \left(1-\varepsilon_g\right)^{1.5}$$

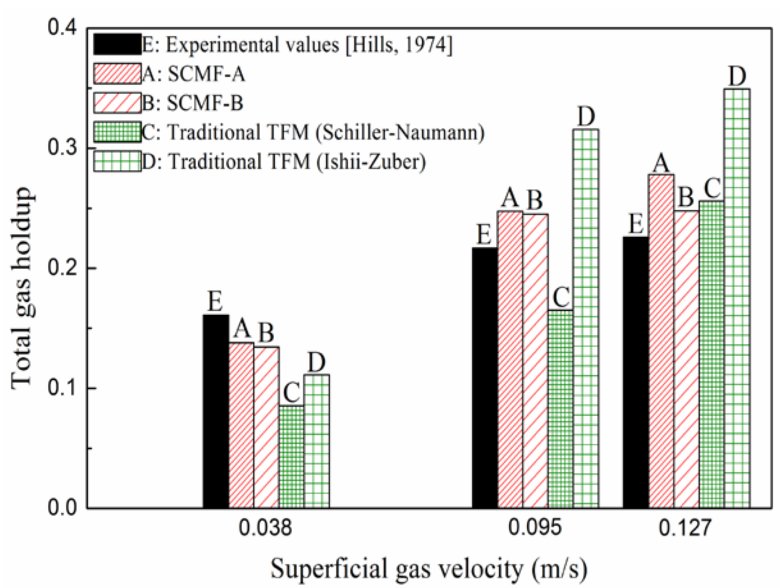
SCMF-B

$$\left(C_D/d_b\right)_L = \begin{cases} 337.90 - 6084.15U_g + 37066.03U_g^2, & U_g \le 0.101 \text{ m/s} \\ 142.22 - 661.62U_g + 897.53U_g^2, & U_g > 0.101 \text{ m/s} \end{cases}$$

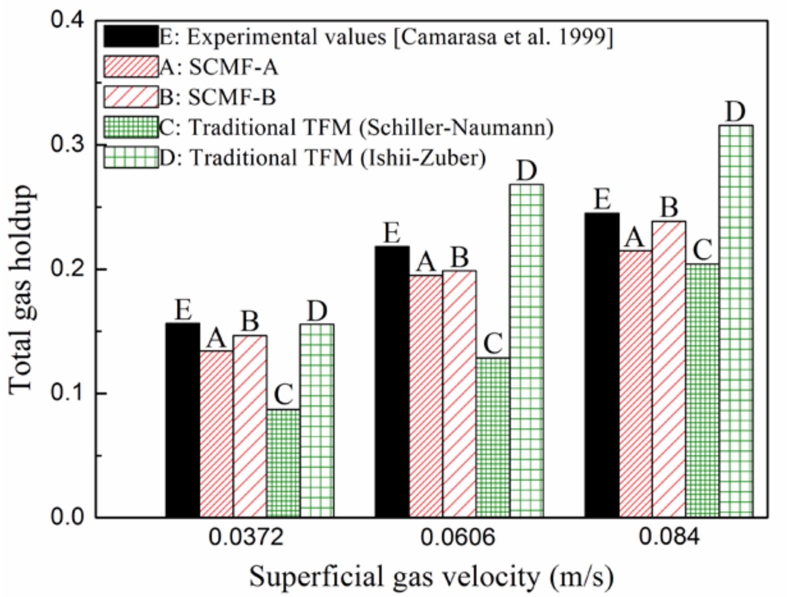
$$\varepsilon_{gs} = F\left(U_{g,L}, f_L, d_L, U_{g,S}, f_S, d_S\right)$$

Comparison between different models: Total gas holdup

Bubble column (Hills, 1974)



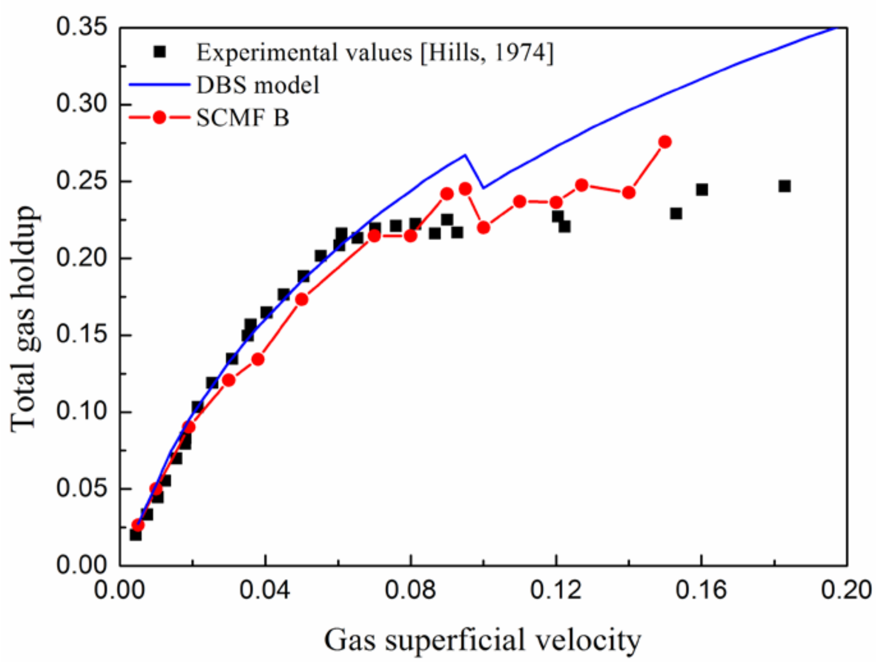
Bubble column (Camarasa, 1999)



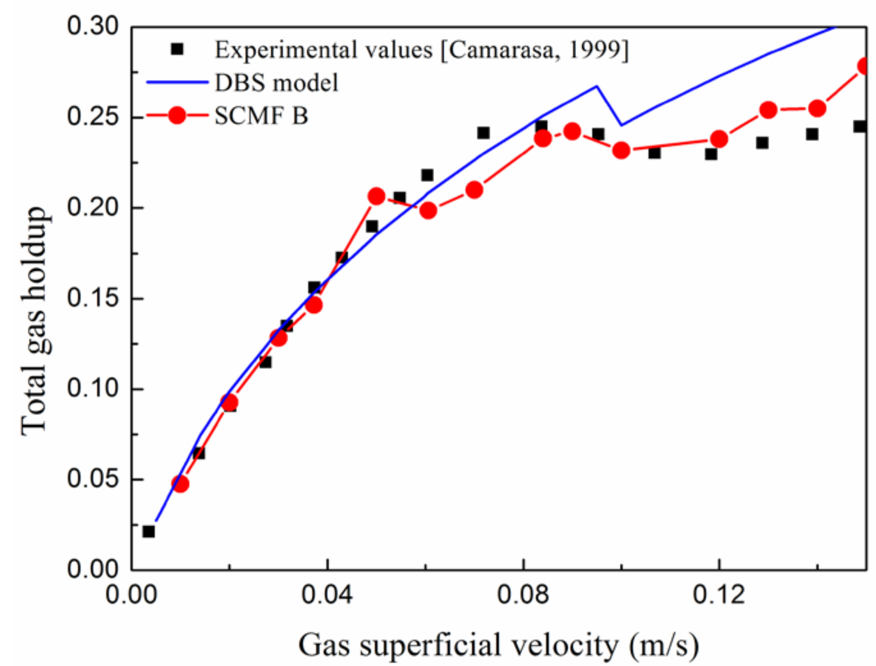
- Ishii-Zuber model over-estimates the total gas holdup at higher Ug
- Schiller-Naumann model under-predicts the total gas holdup at lower Ug

Simulation with the SCMF-B model (Total gas holdup)

Bubble column (Hills, 1974)



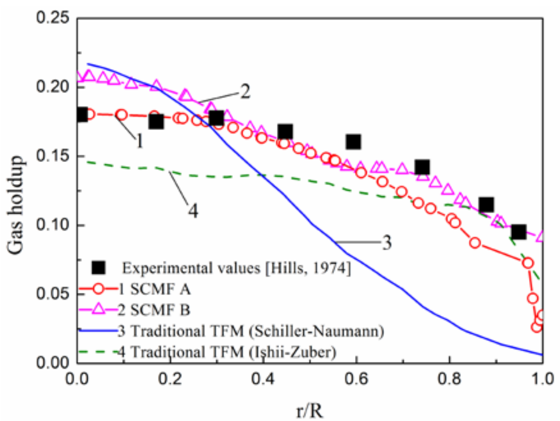
Bubble column (Camarasa, 1999)



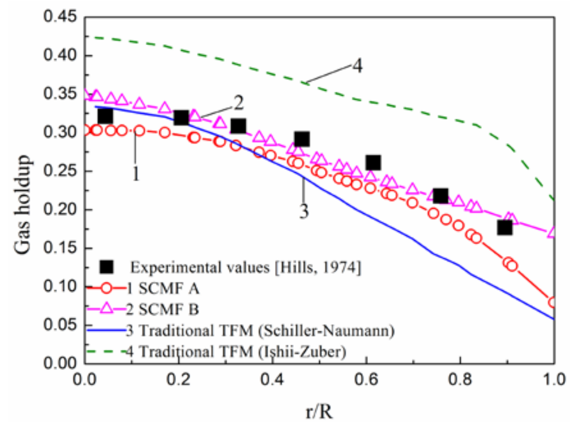
The SCMF-B model can reproduce the plateau or shoulder of the gas holdup curve

Comparison between SCMF-A, B and other models (Hills column)

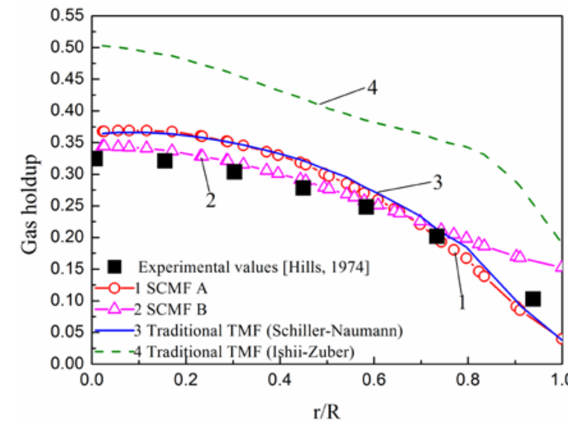
Radial profile of gas holdup



Ug=3.8 cm/s

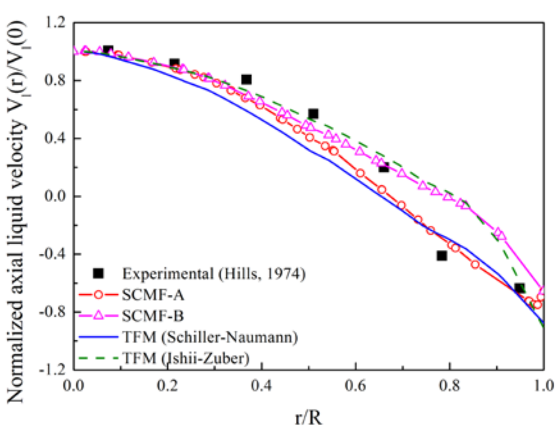


Ug=9.5 cm/s

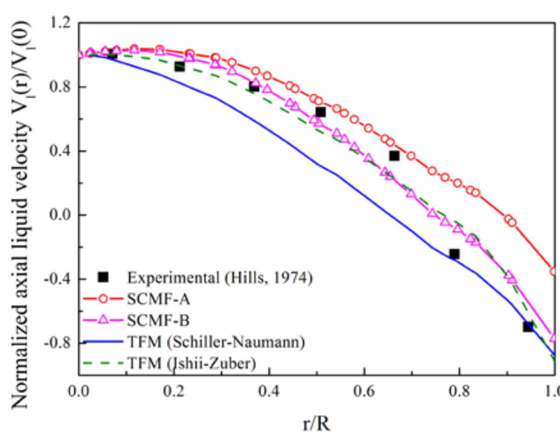


Ug=12.7 cm/s

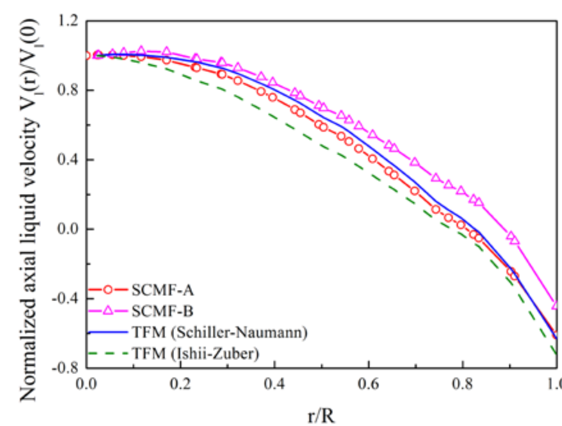
Radial profile of liquid axial velocity



Ug=3.8 cm/s



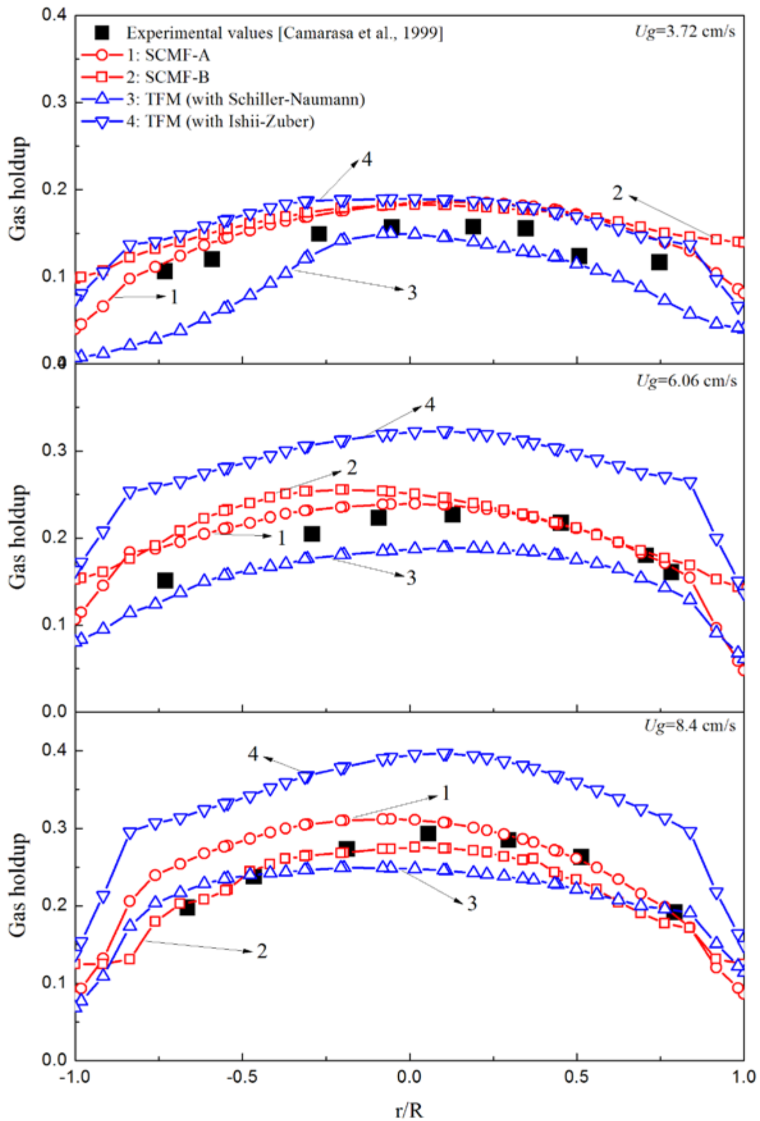
Ug=9.5 cm/s



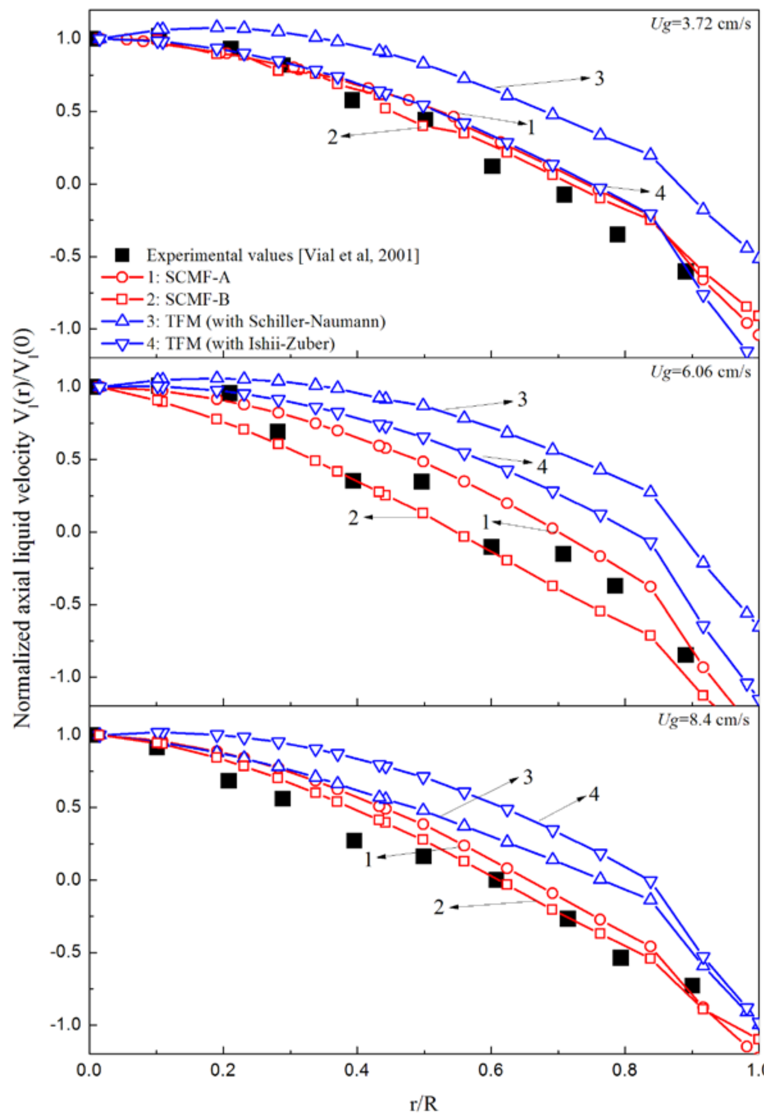
Ug=12.7 cm/s

Comparison between SCMF-A, B and other models (Camarasa column)

Radial profile of gas holdup



Radial profile of liquid axial velocity



SCMF-B

Ug=0.038m/s

Ug=0.095m/s

Ug=0.127m/s

Evolution from SCMF-A to SCMF-B

SCMF-A model
1. Conservative equations for gas and liquid;
2. Inlet flow rate U_g ;
3. Drag coefficient $(C_D/d_b)_T$ extracted from DBS model.

↓ Change the physical properties of two "fluids" to that of dilute and dense phases

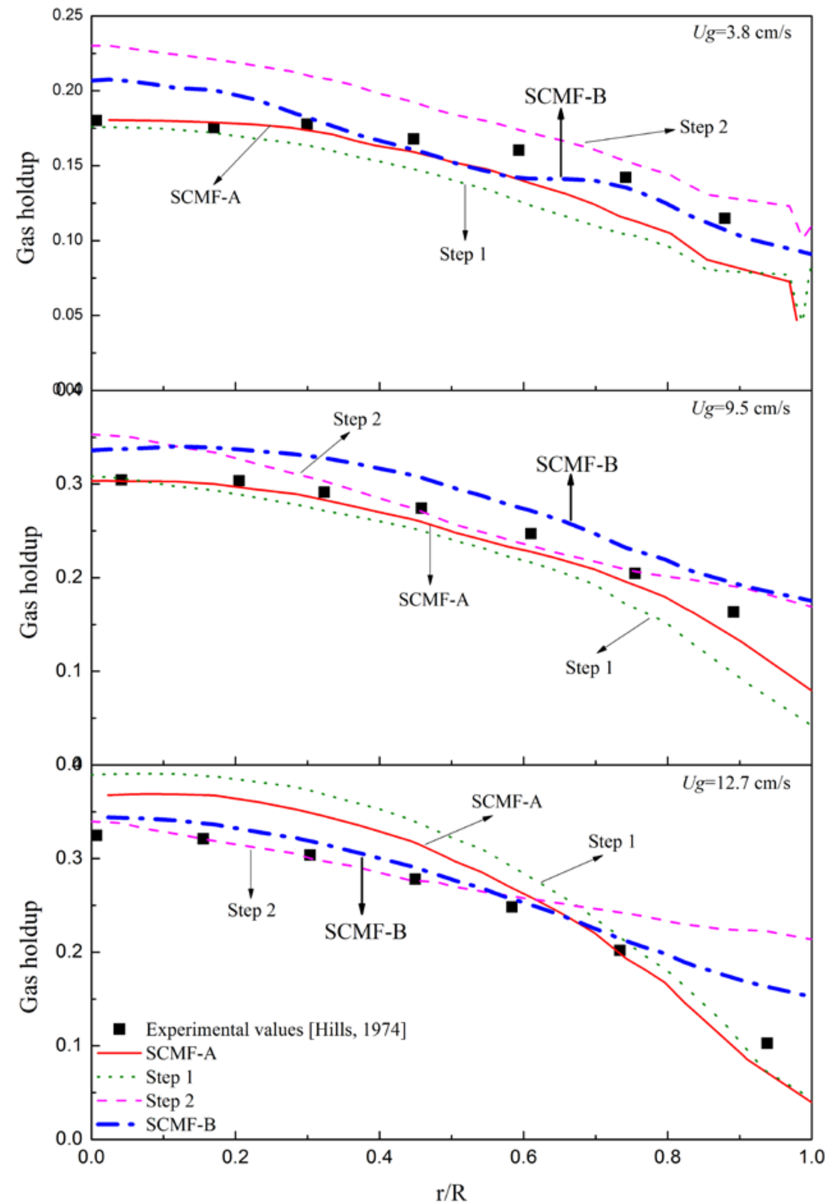
Step 1
1. Conservative equations for two "fluids" ;
2. Inlet flow rate U_g;
3. Drag coefficient $(C_D/d_b)_T$ extracted from DBS model.

↓ Change the inlet flow rate to $U_{g,L}$.

Step 2
1. Conservative equations for two "fluids" ;
2. Inlet flow rate $U_{g,L}$;
3. Drag coefficient $(C_D/d_b)_T$ extracted from DBS model.

↓ Change the drag coefficient to $(C_D/d_b)_L$

SCMF-B model
1. Conservative equations for two "fluids" ;
2. Inlet flow rate $U_{g,L}$;
3. Drag coefficient $(C_D/d_b)_L$ extracted from DBS model.



Conclusions and Prospects

- ***Stability condition***

supply a new constraint for gas-liquid complex flow in addition to mass and momentum conservative equations

- ***Regime transition***

can be physically understood via the jump change of the minimum point of micro-scale energy dissipation in the 3D space of structure parameters.

- ***Stability-constrained multi-fluid CFD approach***

  - **are superior to traditional TFMs with empirical drag correlations:**
    Without the need to adjust correction factors
    Suitable for low, intermediate and higher gas flow rates
    Can capture the plateau or shoulder of the gas holdup curve

  - **Each SCMF model has its strength and weakness by comparison.**
    SCMF-A is better for lower and much higher flow rates.
    SCMF-B is better for prediction of overall gas holdup / at relatively higher gas flow rate / the wall region for lower gas velocity.

  - **may offer a closure for CFD and may be of significance to the fundamental of multiphase flow.**

Recent publication

1. Yang, N* (2012) A multi-scale framework for CFD modeling of multi-phase complex systems based on the EMMS approach. *Progress in Computational Fluid Dynamics*, 12(2-3), 220-229.

2. Yang, N*, Wu, Z., Chen, J, Wang, Y., Li, J (2011) Multi-scale analysis of gas-liquid interaction and CFD simulation of gas-liquid flow in bubble columns. *Chemical Engineering Science*, 66(14), 3212-3222.

3. Yang, N*, Chen, J., Ge, W., Li, J. (2010). A conceptual model for analysing the stability condition and regime transition in bubble columns. *Chemical Engineering Science*. 65, 517-526, 2010.

4. Xiao, Q., Yang, N.*, Li, J., (2013). Stability-constrained multi-fluid CFD models for gas-liquid flow in bubble columns. *Chemical Engineering Science*. 100, 279-292.

5. Shu, S., Yang, N.*, (2013). Direct numerical simulation of bubble dynamics using phase-field model and lattice Boltzmann method. *Industrial and Engineering Chemistry Research*. DOI: 10.1021/ie303486y

Thank you for your attention