2008 International ANSYS Conference

Computational Modeling of Industrial Biofuel Reactors

Jaydeep Kulkarni   Presenter: Genong Li
Technical Account Manager
ANSYS, Inc.

Outline

- Bioreactor design overview
- Benefits of computer modeling
- Case Study : Airlift reactors
  - Multiphase modeling of gas-liquid mixture
  - Prediction of bubble size distribution, mass transfer coefficient and gas hold-up

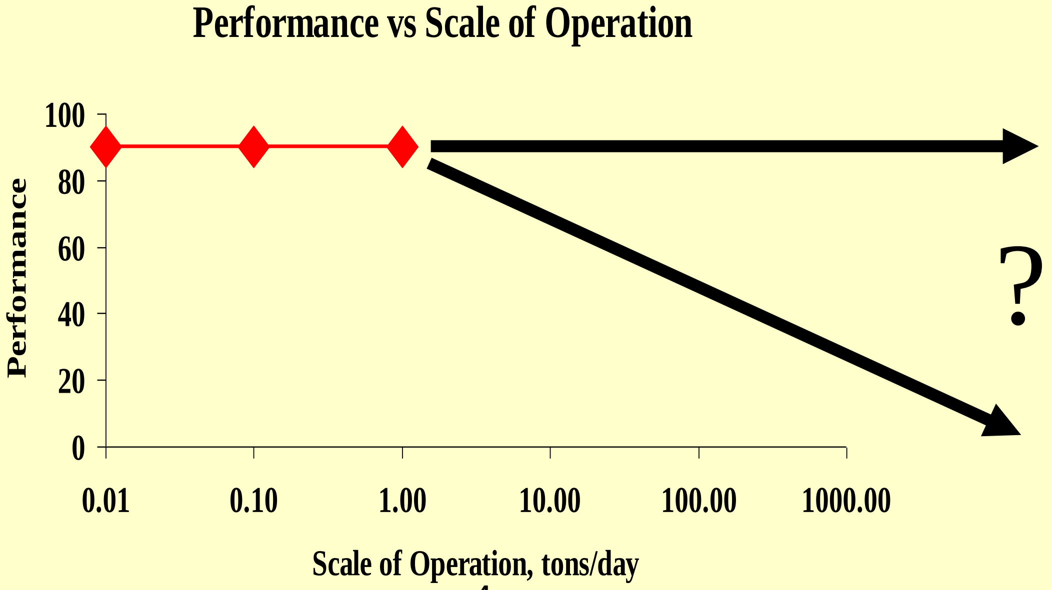
Bioreactor designs

- Bioreactors will be integral to the development of existing high-value products and the replacement of existing chemical-based commodity processes – (Recent Chemical Engineering Progress article)

- Different types of Bioreactors:
  - Stirred tank with baffles and agitators
  - Airlift reactor systems
    - Concentric draft-tube design
    - External-loop airlift design
  - Others such as trickle-bed reactors with immobilized enzymes

Benefits of computer modeling

- Low cost and faster turnaround time for new designs
- No process down-time while analyzing new designs
- Detailed physical insight and visualization
  - More educated design process
  - Minimizing risk of a design failure
- Staying ahead of competition!



Case study: Airlift reactors

- Airlift reactors are suitable for large-scale operations with increased output:
  - Simple design with no moving parts – less maintenance, less risk of defects and easier sterilization
  - Lower shear rate for greater flexibility
  - Large specific interfacial contact-area with low energy input
  - Well-controlled flow and efficient mixing
  - Increased mass transfer due to enhanced oxygen solubility achieved in large tanks with greater pressures

CFD and Bioreactor Design

- In many biological processes, the rate of product formation can be enhanced by increasing the rate of transport of a limiting nutrient.
- For aerobic bioreactions, the rate of oxygen transfer to the cells is usually the limiting factor.
- Oxygen transfer can be studied by measuring/ predicting gas-holdup and the liquid volumetric mass transfer coefficient.
- Scale-up and design must meet oxygen transfer requirements while keeping shear rates low and controlled flow.

Predicting oxygen transfer using computational fluid dynamics (CFD)

- The complex flow characteristics in bioreactors are caused by the existence of bubbles and their motion.
- Multiphase flow models in ANSYS CFD products (ANSYS FLUENT and ANSYS CFX) can be used in conjunction with population balance methods to predict bubble size distributions.
- Bubbles frequently break-up and coalesce due to interactions with turbulent eddies, giving rise to a distribution of bubble sizes.
- It is important to account for this phenomenon for accurately determining interfacial areas for heat and mass transfer rates.

CFD model description

- The air-water system is considered as a two-phase multiphase flow using a multi-fluid Eulerian model.
    - In this approach one set of momentum equations are solved for each phase (gas and liquid)
    - Volume fractions characterize equation set for each phase
    - Coupling among phases achieved through interphase exchange terms

- The gas phase is assumed to be composed of n bubble classes and a population balance equation is solved for each bubble class with birth and death terms due to breakup and coalescence.

- The drag for the secondary (gas) phase is based on a Sauter-mean diameter calculated from the distribution of bubble classes.

- The secondary phase and the n bubble classes share the same velocity field.

Euler – Euler model equations

- Continuity:

$$\frac{\partial}{\partial t}\alpha_q\rho_q + \nabla\cdot\left(\alpha_q\rho_q\vec{u}_q\right) = \sum_{p=1}^{n}\dot{m}_{pq}$$

- Momentum for qth phase:

$$\underbrace{\frac{\partial}{\partial t}\left(\alpha_q\rho_q\vec{u}_q\right)}_{\text{transient}} + \underbrace{\nabla\cdot\left(\alpha_q\rho_q\vec{u}_q\vec{u}_q\right)}_{\text{convective}} = \underbrace{-\alpha_q\nabla p}_{\text{pressure}} + \underbrace{\alpha_q\rho_q\vec{g}}_{\text{body}} + \underbrace{\nabla\cdot\bar{\bar{\tau}}_q}_{\text{shear}} + \sum_{p=1}^{n}\left(\underbrace{\vec{R}_{pq}}_{\substack{\text{interphase}\\\text{forces}\\\text{exchange}}} + \underbrace{\dot{m}_{pq}\vec{u}_q}_{\substack{\text{interphase}\\\text{mass}\\\text{exchange}}}\right) + \alpha_q\rho_q\underbrace{\left(\vec{F}_q + \vec{F}_{lift,q} + \vec{F}_{vm,q}\right)}_{\substack{\text{external, lift, and}\\\text{virtual mass forces}}}$$

- The interphase exchange forces are expressed:

$$\vec{R}_{pq} = K_{pq}\left(\vec{u}_p - \vec{u}_q\right)$$

Population Balance model

- The population balance equation is solved along with the E-E model in ANSYS FLUENT software

- Volume fraction of each bubble class i is governed by

$$\frac{\partial \alpha \rho_i f_i}{\partial t} + \nabla \cdot \left(\alpha \rho_i \bar{u}_d \right) f_i = S_i$$

- The source terms in the equations correspond to the birth and death terms of the population balance equation

$$S_i = B_{Breakup} - D_{Breakup} + B_{Coalescence} - D_{Coalescence}$$

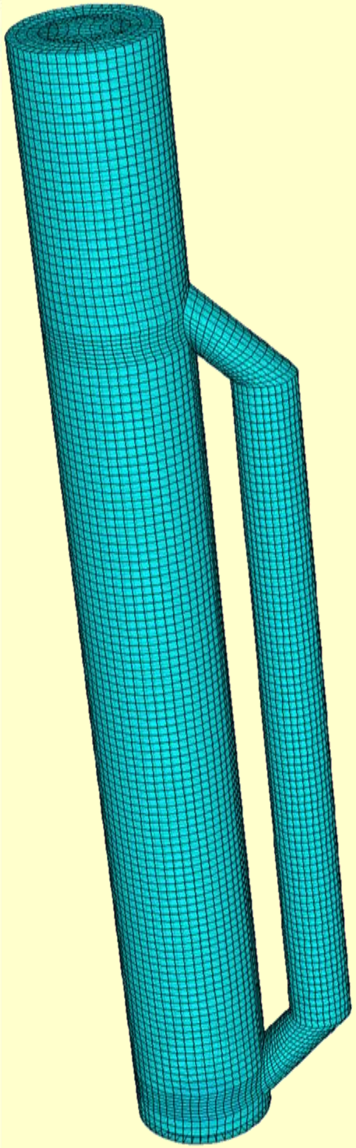
Bubble breakup and coalescence

- Breakup:
  - Bubble breakup models are from a theoretical model by Svendsen and Luo (1996)
  - Bubble breakup is analyzed in terms of bubble interactions with turbulent eddies
  - The turbulent eddies increase the surface energy of the bubbles through deformation
  - Breakup occurs if the increase in surface energy is beyond a critical value
  - The model contains no adjustable parameters

- Coalescence:
  - Bubble Coalescence model is taken from Prince and Blanch (1990)
  - Bubble coalescence is modeled by considering bubble collisions due to turbulence, buoyancy and laminar shear
  - The model is a combination of collision frequency and collision probability

Airlift geometry & numerical conditions

- Airlift reactor geometry and experimental conditions taken from Kawase and Hashimoto (1996)[1] to allow comparison of results
- 23,000 hexahedral Cells modeling 180º of the 3D geometry
- Superficial gas velocities studied are for 0.01 cm/s, 0.02 cm/s and 0.03 cm/s
- Dispersed phase K-ε turbulence Model is used.

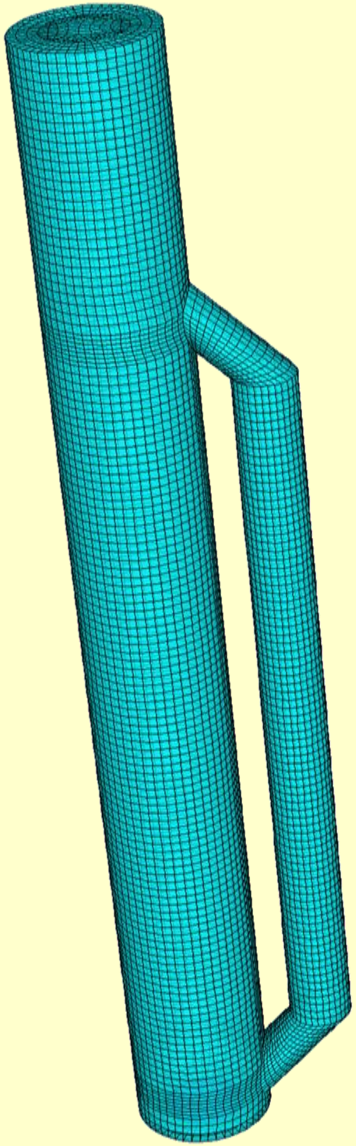


[1] Yoshinori Kawase and Norihisa Hashimoto. J. Chem. Tech. Biotechnol. (1996).

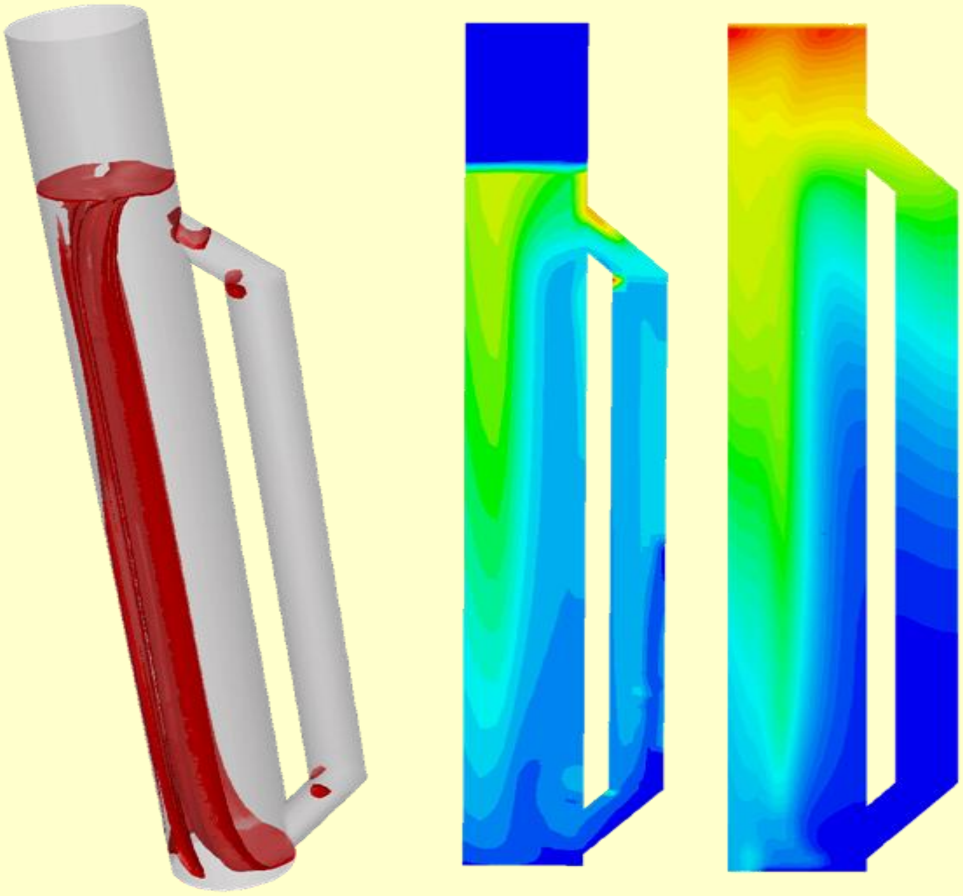
Airlift geometry & numerical conditions

- Breakup and coalescence was modeled by considering a discrete distribution of 9 bubble classes.
- For comparison purposes the calculations were also run for single size bubble without accounting for breakup and coalescence.

[1] Yoshinori Kawase and Norihisa Hashimoto. J. Chem. Tech. Biotechnol. (1996).



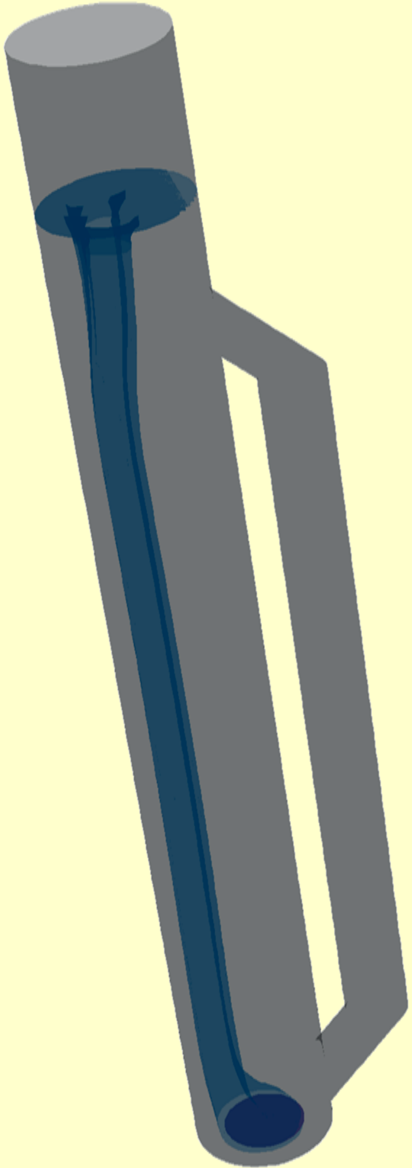
CFD results – phase mixing



L M R

- The air-water interface (L), bubble size distribution (M), and oxygen concentration (R)

CFD results – gas hold-up



- Riser gas holdup (ϕ_{gr}) is calculated as the average volume of gas in the riser section divided by the riser volume (without the freeboard region)

$$\phi_{gr} = \langle \alpha \rangle = 0.035$$

- Volumetric mass transfer co-efficient is calculated as the product of liquid-phase mass transfer co-efficient (KL) and the specific surface area a.

CFD results: mass transfer coefficient

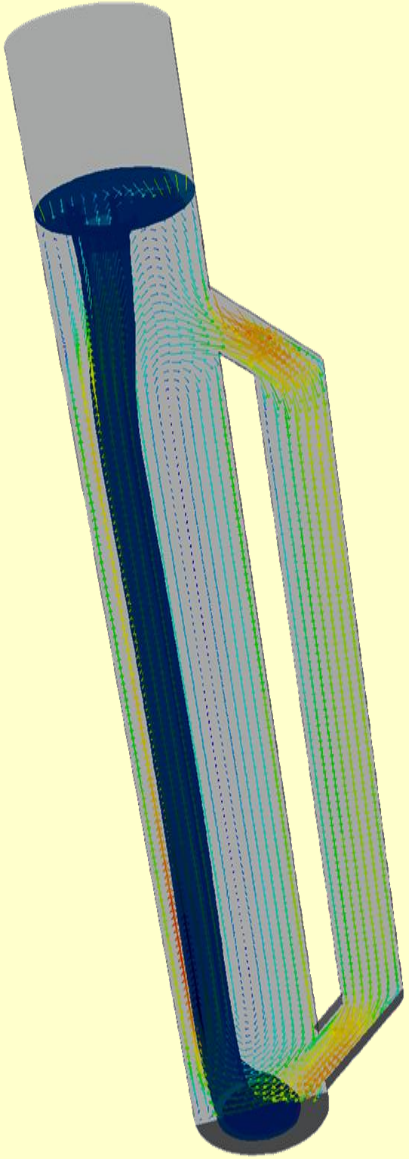
- KL is obtained from the basis of Higbie’s penetration theory as:

$$K_L = \frac{2}{\sqrt{\pi}} \sqrt{D} \left\{ \frac{\varepsilon_L \rho_L}{\mu_L} \right\}^{0.25}$$

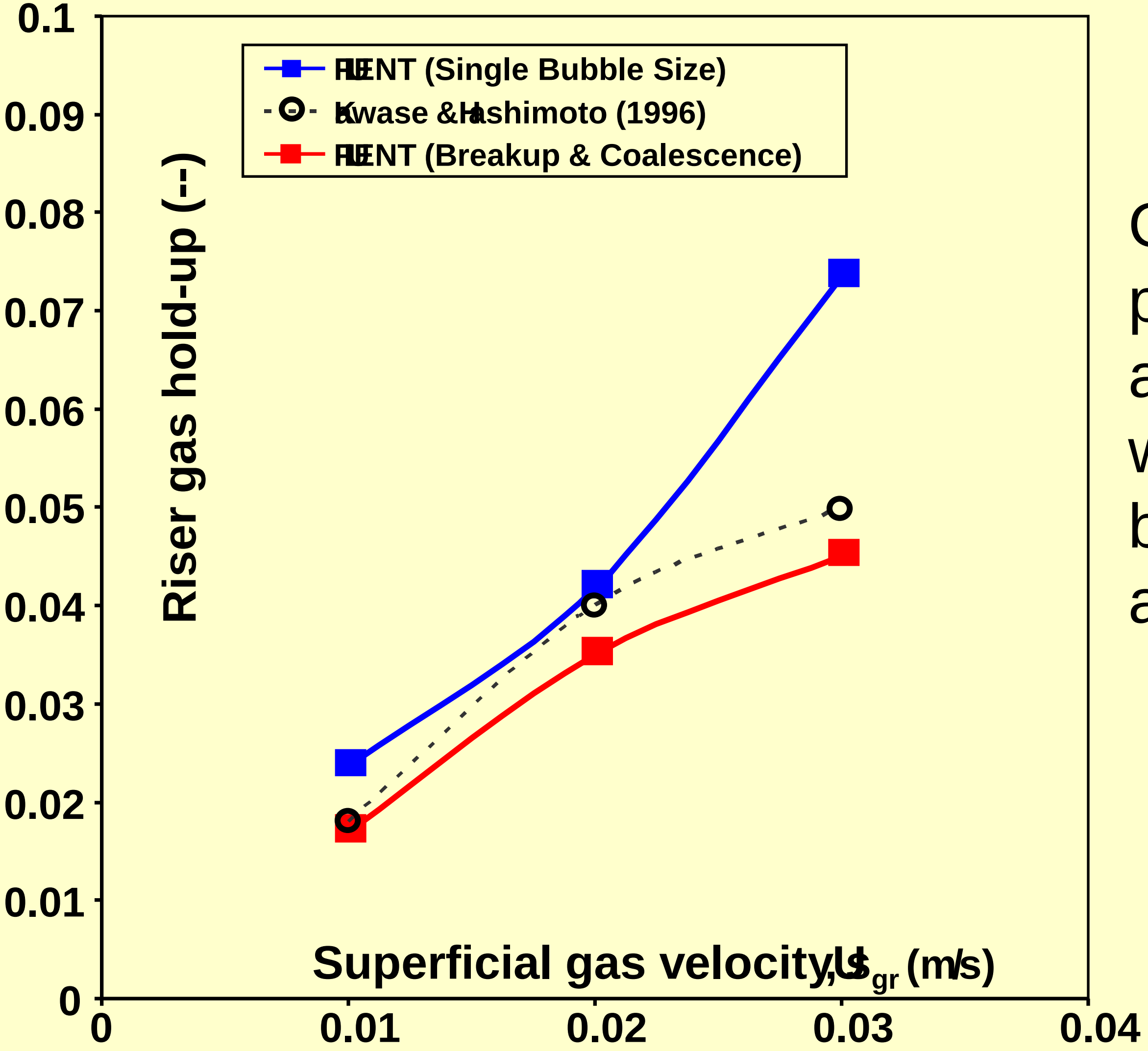
  - ε_L is the water turbulent dissipation rate is predicted from CFD in the above correlation.
- The interfacial area is obtained from the predicted bubble size distribution as:

$$a = \sum_i \frac{6\alpha_i}{d_i}$$

- KLa=0.34 s-1 for air superficial velocity of 0.02 m/s.

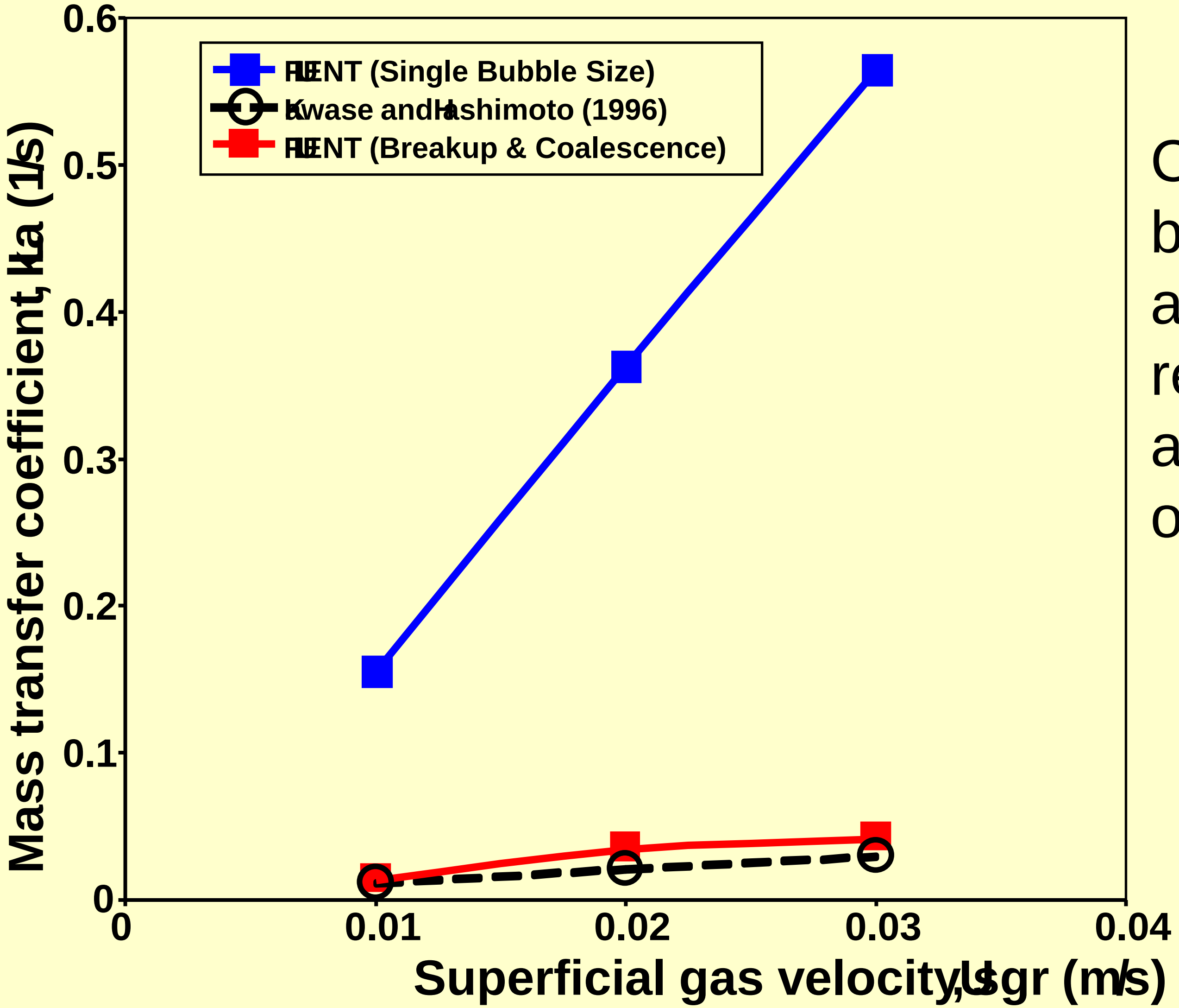


Gas holdup comparisons



Gas hold-up is predicted accurately even without considering bubble break-up and coalescence.

Mass transfer rate comparisons



Consideration of bubble break-up and coalescence required for accurate prediction of mass transfer

Summary of comparisons

Superficial gas velocity (m/s)	Riser Gas Holdup			Liquid Mass Transfer Coefficient (1/s)		
	Kawase & Hashimoto (1996)	FLUENT results		Kawase & Hashimoto (1996)	FLUENT results	
		Single bubble size	Breakup & & Coalescence		Single bubble size	Breakup & &
0.01	0.018	0.0236	0.017	0.011	0.1552	0.013
0.02	0.04	0.0418	0.035	0.02	0.3627	0.034
0.03	0.05	0.0735	0.045	0.029	0.5646	0.041

Conclusions

- Airlift reactor investigated using computational methods
- Good agreement between numerical predictions and experiments
- Computational Modeling can be used to improve yields and minimize design costs