CFD Reactor Modelling

Case Study

Development of CFD model for design, optimisation and scale up of three-phase bubble column reactor with boiling solvent.

Problem

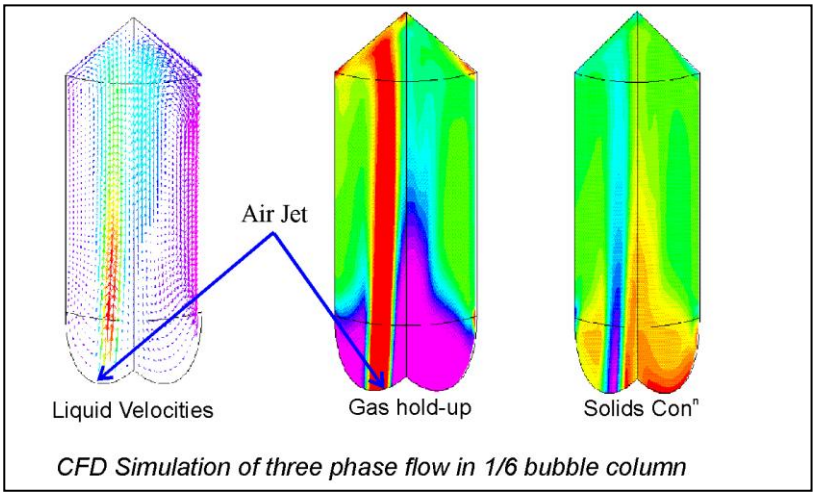
Bubble column reactor design, optimisation and scale up required before building a plant. The process is highly complex three-phase exothermic reaction with boiling solvent and high gas flow velocities, making conventional design and scale-up approaches difficult.

Need

Predictive design, optimisation and scale up tool, capable of accounting for complex three-phase phenomena, to evaluate effects of changing different operational parameters on productivity.

Solution

- Desk and physical model studies to provide data for CFD model construction
- Stepwise construction of CFD model with increasing levels of complexity



CFD Simulation of three phase flow in 1/6 bubble column

Benefits

Predictive validated design model:

- Accounts for three-phase (gas/liquid/solid) mixing and influence of solvent evaporation on simulated flow patterns.
- Facilitates optimised column design and safe, fast and cost-effective exploration of different operational scenarios, minimising pilot plant trials.

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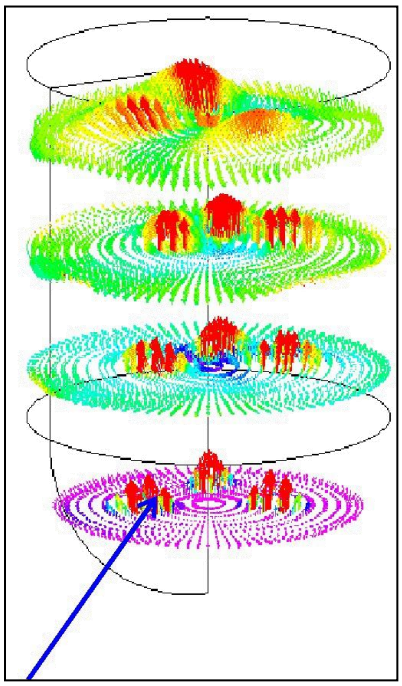
Liquid flow patterns in bubble column



Gas Jet Inlet

Methodology and Results

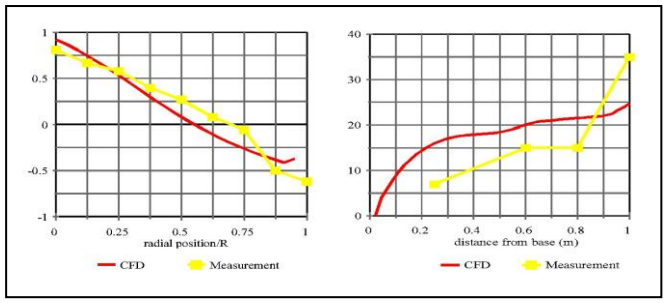
Stage 1

Desk study:

- Assessed complexity of problem & evaluated existing reactor performance
- Designed physical model study to maximise information from measured data
- Physical model study provided data for CFD model construction & testing

Stage 2

- CFD model developed in steps with increasing levels of complexity: single phase liquid flow, tow phase (bubble/liquid) flow and finally three phase (bubble/liquid/solid)
- Three phase flow simulated, and predicted gas hold-up compared with experimental data from physical model and client's existing production scale reactor.
- Three phase flow simulated for full scale column with and without solvent evaporation
- Significance of effects of solvent evaporation due to exothermic reaction evaluated



Liquid Velocity induced by air injection into liquid

Gas Hold-up

BHR Group's Experience

BHR Group is an international centre of fluid mixing expertise and knowhow in the design, optimisation and scale up of chemical reactors for single-phase, two-phase and multiphase processes. Expertise in CFD modelling, chemical engineering and chemistry is backed by unrivalled pilot and production-scale experimental facilities for model validation.

Please contact us for more information or visit our website. P-06

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