A 1D Combined Multifluid-Population Balance Model for the Simulation of Batch Bubble Columns

TECHNISCHE UNIVERSITÄT KAISERSLAUTERN

Laboratory of Reaction and Fluid Process Engineering
Prof. Dr.-Ing. Erik von Harbou

F. Breit[1], A. Mühlbauer[1], E. von Harbou[2], M. W. Hlawitschka[3], H.-J. Bart[1]

[1]Lehrstuhl für Thermische Verfahrenstechnik, Technische Universität Kaiserslautern
[2]Laboratory of Reaction and Fluid Process Engineering, Technische Universität Kaiserslautern
[3]Institut für Verfahrenstechnik, Johannes-Kepler-Universität Linz

Motivation

Bubble columns are widely used as multiphase reactors for gas-liquid reactions in industrial applications.

It is important for the **design engineer** to be able to determine the general **influence** of the **geometry** (e.g. diameter and height) and the **process conditions** (e.g. power input) on the behavior of the reactor at an early stage of **process development**. Thus a model is needed that should be:

- **Fast** and **reliable**;
- Incorporates **couplings** between the **fluid dynamics**, the **population balance equation** (PBE) and the **thermodynamics**;
- **Easy** to calibrate.

Mathematical Model

Dispersed gas phase from the kinetic theory approach with size resolution (KTAWSR)[1]:

Population Balance Equation:

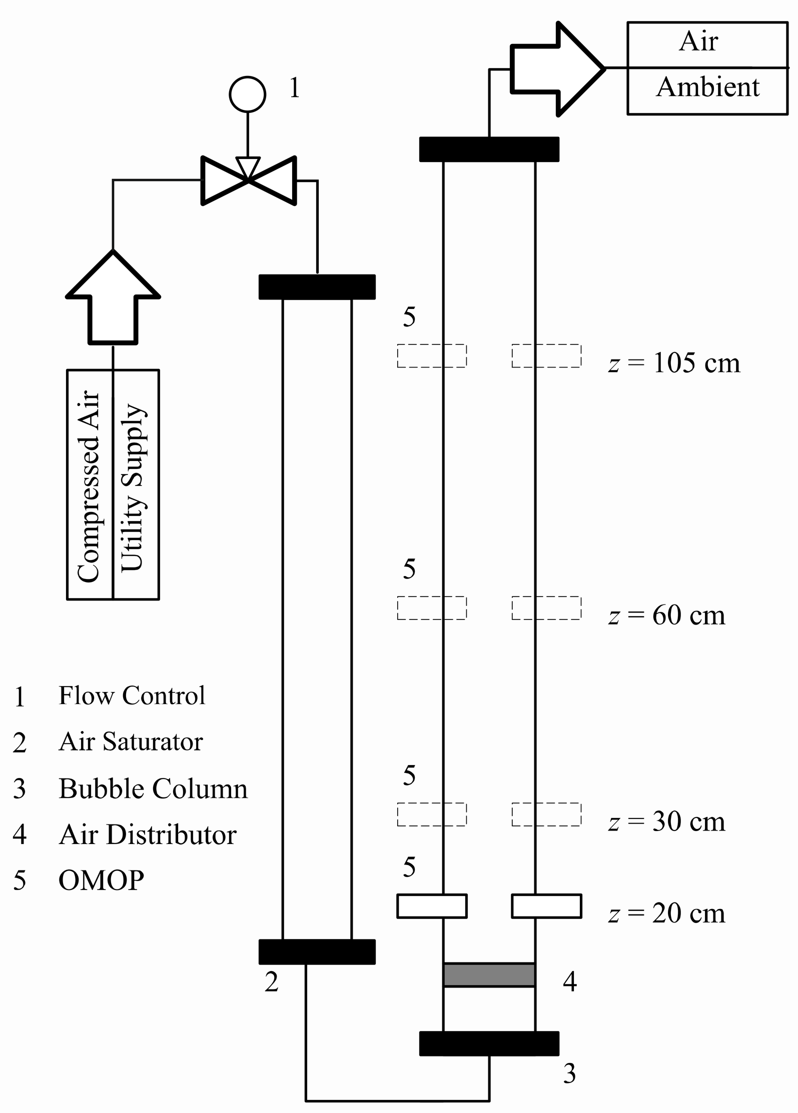
$$\frac{\partial}{\partial z}\left[u_\mathrm{d}(d_\mathrm{d},z)q_\mathrm{d,m}(d_\mathrm{d},z)\right]-\left(\frac{q_\mathrm{d,m}(d_\mathrm{d},z)u_\mathrm{d}(d_\mathrm{d},z)}{\rho_\mathrm{d}(z)}\frac{\partial\rho_\mathrm{d}(z)}{\partial z}\right)-\frac{3}{d_\mathrm{d}}\dot{d}_\mathrm{d}(d_\mathrm{d},z)(d_\mathrm{d},z)$$
$$+\frac{\partial}{\partial d_\mathrm{d}}\left[\dot{d}_\mathrm{d}(d_\mathrm{d},z)q_\mathrm{d,m}(d_\mathrm{d},z)\right]=-B_\mathrm{D}(d_\mathrm{d},z)+B_\mathrm{B}(d_\mathrm{d},z)-C_\mathrm{D}(d_\mathrm{d},z)+C_\mathrm{B}(d_\mathrm{d},z)$$

Momentum:

$$u_\mathrm{d}(d_\mathrm{d},z)q_\mathrm{d,m}(d_\mathrm{d},z)\frac{\partial u_\mathrm{d}(d_\mathrm{d},z)}{\partial z}+\dot{d}_\mathrm{d}(d_\mathrm{d},z)q_\mathrm{d,m}(d_\mathrm{d},z)\frac{\partial u_\mathrm{d}(d_\mathrm{d},z)}{\partial d_\mathrm{d}}=-\frac{q_\mathrm{d,m}(d_\mathrm{d},z)}{\rho_\mathrm{d}(z)}\frac{\partial p(z)}{\partial z}$$
$$+\frac{\partial}{\partial z}\left[\frac{q_\mathrm{d,m}(d_\mathrm{d},z)}{\rho_\mathrm{d}(z)}\mu_\mathrm{d}\frac{\partial u_\mathrm{d}(d_\mathrm{d},z)}{\partial z}\right]-q_\mathrm{d,m}(d_\mathrm{d},z)g+m_\mathrm{d}(d_\mathrm{d},z)$$

Continuous Liquid phase from the mutlifluid model

Experimental Setup



Measurement of the:

- **Integral gas holdup**
- **Bubble size distribution (BSD)**

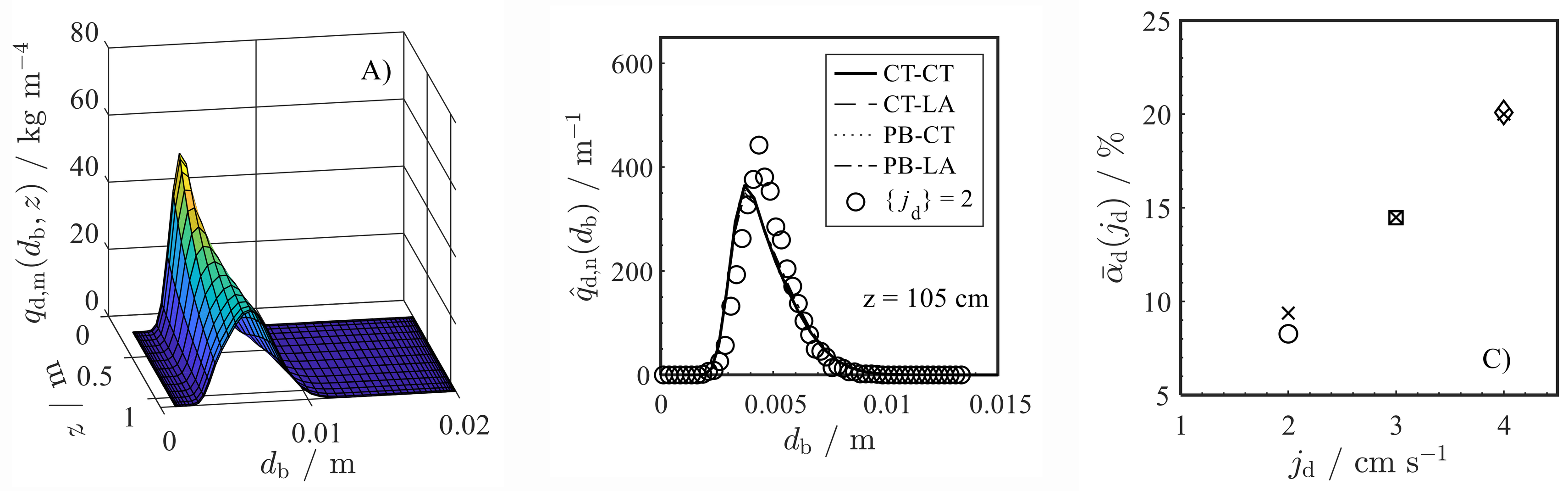
at three gas volume fluxes j_d = (2.0, 3.0, 4.0) cm s^{-1}

at four axial positions

z = (20, 30, 60, 105) cm

in a **DN100** batch **water-air** bubble column.

Results



- **Continuous representation** of the BSD in d_b and z.
- The exp. BSD are **well reproduced** through calibration.
- **Various breakage** and coalescence models give similar results.
- New approach for the calculation of integral gas holdup could be **predictively confirmed**.

Conclusion

- 1D steady-state **combined multifluid-PBE** model is able to describe a batch BC up to the **transition regime**.
- **Fast** parameter calibration, simulation and sensitivity analysis are possible.
- Reliable **deep insights** into complex multiphase systems.
- The developed model represents a **valuable tool** in process development.

Future Research

- Further test of the **scalability** of the calibrated parameters.
- Extension to **reactive systems**.
- Extension to **other reactor types**.

[1] J. Solsvik, H.A. Jakobsen (2014), J. Dispers. Sci. Technol. 35(11), 1611–1625.

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