CFD: a design and scale-up tool for multiphase reactors
van Baten, J.M.

Citation for published version (APA):
van Baten, J. M. (2000). CFD: a design and scale-up tool for multiphase reactors

General rights
It is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), other than for strictly personal, individual use, unless the work is under an open content license (like Creative Commons).

Disclaimer/Complaints regulations
If you believe that digital publication of certain material infringes any of your rights or (privacy) interests, please let the Library know, stating your reasons. In case of a legitimate complaint, the Library will make the material inaccessible and/or remove it from the website. Please Ask the Library: http://uba.uva.nl/en/contact, or a letter to: Library of the University of Amsterdam, Secretariat, Singel 425, 1012 WP Amsterdam, The Netherlands. You will be contacted as soon as possible.
Chapter 1

Introduction

Bubble column reactors operated in industry have several distinguishing features: (1) large column diameters are involved, ranging to 6 m, (2) high superficial gas velocities, in the 0.1 – 0.4 m/s range, are usually used, (3) the system pressure can range to 6 MPa and (4) the liquid phase often consists of a non-aqueous hydrocarbon mixture (Krishna et al., 1996). Laboratory studies on bubble column hydrodynamics are usually carried out with the air-water system, at ambient pressure conditions, in columns that are smaller than say 0.5 m in diameter (Deckwer, 1992). Even for the air-water system, available literature correlations give significantly different results (for details of the correlations see, the companion thesis of Urseanu, 2000). This is demonstrated by the predictions of the total gas holdup and the centre-line liquid velocity as a function of the superficial gas velocity and column diameter; see Figures 1 and 2. Only two correlations plotted in Fig. 1 anticipate that the gas holdup decreases with increasing column diameter. We see from Fig. 2 (b) that the predictions of the centre-line velocity for a bubble column of diameter 6 m diameter operating at $U = 0.3$ m/s varies between 0.9 and 4.5 m/s. This represents a variation of a factor of five and so there is a clear need for a reliable scale up strategy.

The objectives of my thesis are:
1. To develop a fundamental understanding of bubble dynamics and the reasons behind the observed scale dependence of bubble columns, and
2. To develop a model which can be used for design and scale up of commercial bubble column reactors,
3. To validate the developed model by comparing simulation results with experimental data, largely generated in our group at the University of Amsterdam, Department of Chemical Engineering.

The models I use for investigating the bubble dynamics and scaling up are based on Computational Fluid Dynamics (CFD). I develop a multi-tiered approach comprising:
- description of single bubble morphology and rise dynamics using the Volume-of-Fluid (VOF) simulation technique,
- modelling of bubble-bubble interactions using VOF simulations,
- development of Eulerian simulation models for design and scale up.

In order to demonstrate the versatility of CFD tools I also show how the ideas and models developed for bubble columns could be extended to describe the hydrodynamics of gas-solid fluid beds, sieve tray distillation columns and liquid flow through the complex geometry of KATAPAK-S.
Fig. 1. Comparison of literature correlations for the total gas holdup $\varepsilon$ for air-water systems in a column of 0.38 m diameter. (a) Variation of $\varepsilon$ with superficial gas velocity for a column of 0.38 m diameter. (b) Variation of $\varepsilon$ with column diameter for a superficial gas velocity of 0.3 m/s. The plotted correlations are: (1) Krishna and Ellenberger (1996), (2) Wilkinson et al. (1992), (3) Zehner (1989), (4) Akita and Yoshida (1973), (5) Bach and Pilhofer (1978), (6) Reilly et al. (1986), (7) Hikita et al. (1980), (8) Hughmark (1967).

Fig. 2. Comparison of literature correlations for the centre-line velocity $V_L(0)$ for air-water systems. (a) Variation of $V_L(0)$ with superficial gas velocity for a column of 0.38 m diameter. (b) Variation of $V_L(0)$ with column diameter for a superficial gas velocity of 0.3 m/s. The plotted correlations are: (1) Ohki and Inoue (1970), (2) Ueyama and Miyauchi (1979), (3) Joshi (1980), (4) Riquarts (1981), (5) Zehner (1986), (6) Nottenkämper et al. (1983), (7) Ulbrecht et al. (1985), (8) Kawase and Moo-Young (1989), (9) Bernemann (1989).
For validation of the developed CFD models, I have relied on the following set of experimental investigations.

1. Investigation of rise velocity of single gas bubbles in liquids, carried out largely by Urseanu (2000). I also contributed to the measurement of single bubble rise velocities in columns of circular cross-section and 2D rectangular columns,

2. Flow visualisation studies of in-line interactions of bubble pairs. These measurements were carried out by Urseanu (2000),

3. Investigation of gas holdup in bubble columns of varying column diameters. The data bank was generated within our group at the University of Amsterdam and published in the theses of Ellenberger (1995), De Swart (1996) and Urseanu (2000),

4. Measurement of centre-line liquid velocities in bubble columns of three different diameters. These measurements were performed by Urseanu (2000),

5. Measurement of the radial distribution of liquid velocity in columns of three different diameters. These measurements were performed by Urseanu (2000),

6. Measurement of the axial dispersion coefficient of the liquid phase in columns of three different diameters. These measurements were performed by Urseanu (2000),

7. Measurement of clear liquid height on rectangular sieve trays. I performed these measurements in collaboration with Dr. J. Ellenberger and Dr. A.P. Higler,

8. Measurement of residence time distribution within the liquid phase of KATAPAK-S. I participated in the measurement programme and helped to analyse the experimental results.

I performed the CFD simulations reported in this thesis on the following platforms (consisting of a total of 9 processors):

1. Silicon Graphics Indigo 2 Workstation, 75 MHz R8000 processor,

2. Silicon Graphics Indigo 2 Workstation, 75 MHz R8000 processor,

3. Silicon Graphics O2 Workstation, 150 MHz R10000 processor,

4. Silicon Graphics Power Challenge Workstation with six R8000 processors, later upgraded to 200 MHz R10000.

All simulations were carried out using a commercial solver CFX 4.1 (later upgraded to 4.2) of AEA Technology, Harwell. The details of the computational models and the numerical approach used are given in the Appendix.

The layout of my thesis is as follows: Chapters 2, 3 and 4 deal with VOF simulations of single bubble rising in liquids and the study of bubble-bubble interactions. In Chapter 4, I also compare the VOF technique with the Kinetic Theory of Granular Flow in order to emphasise the analogies between bubble rise in liquids and powders.

Chapters 5, 6 and 7 develop a three-phase Eulerian description of bubble columns for simulation, design and scale up. Chapter 8 extends the ideas for bubble columns to gas-solid fluid beds.

Chapter 9 and 10 develop a CFD model for description of sieve tray hydrodynamics.

Chapter 11 uses CFD techniques to study flow of liquid through a packed bed in the complex geometry of KATAPAK-S.

Chapter 12 summarises the major conclusions of this thesis.

The chapters have been written in more-or-less self-contained fashion and have been published as individual papers. Therefore, some degree of overlap exists.