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Simulation and experimental validation of reactive bubble column reactors

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HIGHLIGHTS

- Laser based measurement technique to determine local hydrodynamics.
- Local data of concentration fields in bubble columns.
- Reactive CFD simulation using Euler-Euler CFD code.
- Validation against own local experimental data at several column heights.

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ABSTRACT

Bubble columns are widespread in chemical process engineering. The overall performance of these reactors relies on the interaction between the hydrodynamics, interfacial mass transfer and chemical reactions. The layout of these columns is commonly based on simplified integral models that are not able to track the complex interactions between the local hydrodynamics and the reactions. Hence, a detailed knowledge about the ongoing interactions is required. The local and temporal evolution of the carbon dioxide (CO_2) chemisorption in aqueous *NaOH* solution in a cylindrical bubble column is investigated. Therefore, local measurements of hydrodynamics, bubble size and velocity, liquid velocity and concentration (pH-value) are done using a high speed PIV/LIF system combined with shadowgraphy. The results are compared to Euler-Euler based computational fluid dynamics simulations that take into account the ongoing reaction.

1. Introduction

The most primitive reactor types for multiphase flows are bubble columns (Deckwer, 1992; Joshi, 2001; Gruber et al., 2015). They are applied intensively as multiphase contactors and reactors in chemical, biochemical and pharmaceutical industries (Mills and Chaudhari, 1997; Kantarci et al., 2005; Kulkarni and Joshi, 2005, 2011). The range of applications includes absorption, catalytic slurry reactions, coal liquefaction, bioreactions, etc. (Shah et al., 1982; Deckwer, 1985). Nevertheless, their numerous designs and internals make a general design procedure until now difficult. The gas is introduced into the column through a single sparger or by multiple spargers that can be located at several column heights in order to reduce locally high gas fractions. The sparger design is critical since it can dominate the overall column performance (Thorat et al., 1998; Kulkarni and Joshi, 2011). The initial bubble size is determined by system properties, gas flow rate and sparger geometry (Kulkarni and Joshi, 2005). After bubble generation, the bubble rises through the column, induces local velocity fluctuations and interacts with other bubbles, resulting in bubble coalescence and breakage. The absorption of gas leads on one hand to a shrinkage of the bubbles, while the reduction of hydrostatic pressure acting on the bubbles in the column could lead on the other hand to a bubble size increase along the column height.

The interaction between the continuous and dispersed phase generates vortices and time dependent swirl structures. This results into different retention times of the gas bubbles and the absorbed solute, which may react in the liquid to further products. As pointed out, reactive bubble columns are generally complex to describe due to the above discussed interactions. Thereby, the bubble diameter distribution is the most critical parameter in the overall performance of the column (Fig. 1).

The design of bubble columns however is still done by modelling the columns based on integral correlations for hold-up, bub-

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Latin symbols

a	specific interface area [m^{-2} m^{-3}]
c	concentration [kmol m^{-3}]
d	diameter [m]
d_c	phase material time derivative for the continuous phase
d_d	phase material time derivative for the dispersed phase
$\vec{g}$	gravitational acceleration [kg m^{-1} s^{-2}]
k_l	mass transfer coefficient [m s^{-1}]
k_m	reaction rate constant [varies]
$\dot{m}$	mass transfer [kg m^{-3} s^{-1}]
p	pressure [Pa]
t	time [s]
$\vec{u}$	velocity [m s^{-1}]
A_{bubble}	bubble interface area [m^2]
C_α	interface sharpening constant
C_D	drag coefficient
C_S	Smagorinsky coefficient
D	diffusion coefficient [m^2 s^{-1}]
E	enhancement factor
Eo	Eötvös number
E_{sh}	shape factor
F	force [N]
H	dimensionless Henry constant
K	drag exchange coefficient [kg m^{-3} s^{-1}]
K_{GG}	equilibrium constant
Re	Reynolds number
S	source term [kg m^{-3} s^{-1}]
$\hat{S}$	mean rate of strain tensor
Sc	Schmidt number
Sh	Sherwood number
T	temperature [K]
V	volume [m^3]
V_{bubble}	bubble volume [m^3]
W	molar mass [kg $kmol^{-1}$]
Y	mass fraction [kg kg^{-1}]
X	empirical formula

Greek symbols

α	volumetric phase fraction
β	stoichiometry coefficient
μ	dynamic viscosity [kg m^{-1} s^{-1}]
μ_{sgs}	turbulent viscosity [kg m^{-1} s^{-1}]
ρ	density [kg m^{-3}]
σ	Interfacial tension [N m^{-1}]
σ_{TD}	Turbulent Schmidt number
ω	reaction velocity [kmol m^{-3} s^{-1}]

Indices

comp	compression
g	gaseous
i	phase
j	chemical species
l	liquid
A	activation
D	drag
VM	virtual mass

Superscripts

*	interface
′	forward reaction
″	reverse reaction

Abbreviations

2T-LIF	2-Tracer Laser Induced Fluorescence
CCD	charge-coupled device
CFD	computational fluid dynamics
PIV	Particle Image Velocimetry
PTV	Particle Tracking Velocimetry

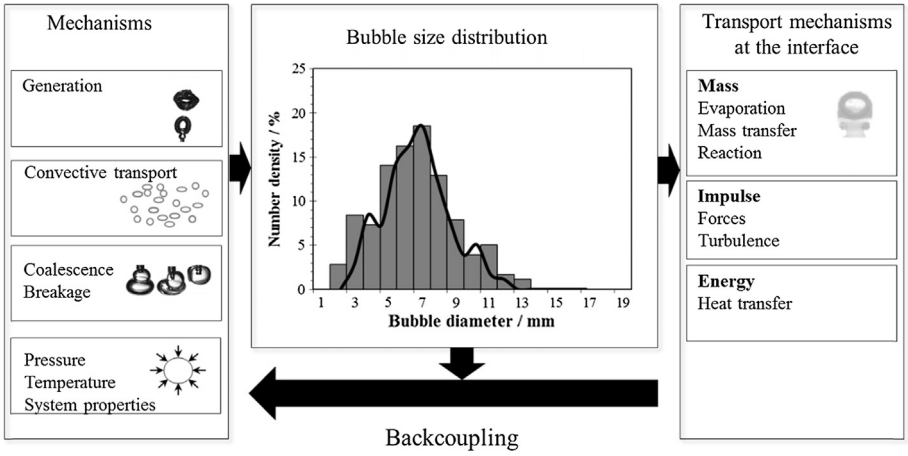

Fig. 1. Interaction of different mechanisms, bubble size distribution and interface transport mechanism (following Gnotke, 2005).

ble size and hydrodynamics, such as via axial dispersion. Appropriate correlations are mainly generated for specific chemical systems (mainly air/water) and for specific column types and thus limit a general scale-up of bubble columns. The hydrodynamic modelling is supported by experiments on various scales. Therefore, single bubble investigations are used to study the bubble rise, mass transfer and binary coalescence. Swarm experiments examine swarm effects at different hold-ups, where final pilot plant experiments reveal the overall performance. These are supported by single equipment investigations, such as the study of the disperser, additional coalescer, and so on. In that respect, spatial and time resolved investigations of the bubble size distribution comes into focus of academia and industrial research to obtain a deeper understanding of the local phenomena. Nevertheless, a better understanding of the local hydrodynamics/mass transfer interaction can only be obtained, when all influencing parameters