An Experimental and Computational Study of Hydrodynamics and Mass Transfer in Gas-Liquid Bubble Columns

Von der Fakultät für Naturwissenschaften
- Department Chemie -
der Universität Paderborn

zur Erlangung des akademischen Grades
Doktor der Naturwissenschaften
- Dr. rer. nat. -

Vorgelegte Dissertation
Von

Houman Shirzadi
M.Sc. in Chemical Engineering
- biotechnology -
aus Teheran

Paderborn 2010

Schriftenreihe Institut für Polymere Materialien und Prozesse

Band 3/2012

Houman Shirzadi

An Experimental and Computational Study of Hydrodynamics and Mass Transfer in Gas-Liquid Bubble Columns

D 466 (Diss. Universität Paderborn)

Shaker Verlag
Aachen 2012

Bibliographic information published by the Deutsche Nationalbibliothek
The Deutsche Nationalbibliothek lists this publication in the Deutsche Nationalbibliografie; detailed bibliographic data are available in the Internet at http://dnb.d-nb.de.

Zugl.: Paderborn, Univ., Diss., 2011

Printed in Germany.

ISBN 978-3-8440-0946-0
ISSN 2191-2025

Shaker Verlag GmbH • P.O. BOX 101818 • D-52018 Aachen
Phone: 0049/2407/9596-0 • Telefax: 0049/2407/9596-9
Internet: www.shaker.de • e-mail: info@shaker.de

Dedicated to my ***Family***

Abstract

In this thesis with the aid of experimental measurements and CFD modelling validations, the hydrodynamics and mass transfer in the gas-liquid bubble columns, have been simulated. For this purpose, the commercial CFD-software ANSYS CFX has been applied.

The experiments have been carried out with a laboratory scale bubble column and could be divided into two distinct parts; first part, studying the hydrodynamics i.e. the axial dispersion coefficient and the gas hold-up inside the bubble column with respect to the different flow rates of gas and liquid phase and the second part, studying the mass transfer i.e. the volumetric mass transfer coefficient, again with respect to the different flow rates.

Following the experimental studies, the respective CFD model with the Eulerian-Eulerian approach and a single sized bubble as the disperse phase was set to simulate the flow field. For this purpose different closure models such as turbulence and drag models have been examined and these results were compared with the experimental data.

Furthermore, a mass transfer model has been developed in order to account for the mass transfer between the phases. For this part of the simulations, the volumetric mass transfer coefficients obtained from the experiments, were set into the CFD model for the numerical calculations. Therefore, the respective experimental flow conditions were applied in the simulations to validate the CFD model. It was observed that the hydrostatic pressure inside the bubble column plays an important role in the mass transfer between the two phases.

Finally, the simulation results show that the Euler model with all its simplifications is still an appropriate and cost effective approach for the numerical simulation of the two phase flow in the bubble column reactors.

Acknowledgements

This thesis would not have been possible, without the support and the guidance of several individuals, who in one way or another contributed their valuable assistance in completion of this study.

First and foremost, my utmost gratitude to my adviser Prof. Dr.-Ing. Hans-Joachim Warnecke, who gave me this opportunity to accomplish my Ph.D. study under his guidance. His intensive support had the major influence on the success of this thesis. Also in addition to all his technical support, I am very grateful for his considerable encouragement and moral support in the time of need.

Next, I would like to express my deepest thanks to Prof. Dr. Dieter Bothe for his support, constructive criticism and his innovative ideas. This thesis would not have come to a successful completion without his valuable guidance.

Here, I would like to show my gratitude to the group members of the Technical Chemistry, especially my dear colleagues and friends; Dr. Bhaskar Bandarapu and Dr. Martin Schmidtke for the great working atmosphere and being open to all technical discussions. Also, my thanks go to Dr. Mike Bobert for all his considerations and the respective administration work, Dr. Hubert Stenner for his efforts and for supporting me in my experimental investigations. I also appreciate the support of Dr. Andreas Alke for providing me a better understanding in some mathematical issues. I would also like to thank the financial support of the German Academic Exchange Service (DAAD) for providing me the scholarships.

I am also very grateful to my current chief, Dr. Martin Dauelsberg for providing me a flexible working atmosphere, so that I could accomplish my thesis beside my job.

I also appreciate all the supports and encouragements from my family members and friends who helped me throughout this work, especially my brother Dr. Houtan Shirzadi, who played a very important role in finding this opportunity and providing me the first initial requirements for a successful start.

Finally, I would like to express my most sincere gratitude and appreciation to my father and my mother who always believed in me and continuously supported and encouraged me in all I did for as long as I remember. I thank you both from the bottom of my heart.

Last, but not least, I would like to dedicate this thesis to my loving wife, Sally Adnani, who always supported me with her unending love and care during all ups and downs of my Ph.D. I would like to appreciate her patience and support, which allowed me to accomplish this thesis.

March 2010 *Houman Shirzadi*

List of Abbreviations and Symbols

Abbreviations

ADM	axial dispersion model
CFD	computational fluid dynamics
C.S.	control surface
C.V.	control volume
DAAD	deutscher akademischer austausch dienst
DNS	direct numerical simulation
DO	dissolved oxygen
FDM	finite difference method
FEM	finite element method
FVM	finite volume method
ip	integration point
LDA	laser doppler anemometry
LES	large eddy simulation
MUSIG	multiple size group
PDE	partial differential equation
PIV	particle image velocimetry
RANS	reynolds averaged navier stokes
SST	shear stress transport
UDS	upwind difference scheme
VOF	volume of fluid

Roman Symbols

Symbol	Description	Dimensions
A	area	m^2
a	gas/liquid interface area per liquid volume	m^2/m^3
C_{cd}	momentum transfer coefficient	-
C_D	drag coefficient	-
C_L	lift coefficient	-
C_{TD}	modifiable coefficient	-
C_{VM}	virtual mass coefficient	-
c	specie concentration	kg/m^3
D	dispersion coefficient	m^2/s
d	diameter	m
F_b	blending function	-
g	gravity	m/s^2
H	Henry's constant	$m\ s^2/kg$
k_L	mass transfer coefficient	m/h
k_La	volumetric mass transfer coefficient	1/h
L	characteristic length	m
l_t	turbulence length scale	m
M	interfacial forces	$kg\ m/s^2$
M^D	interphase drag force	$kg\ m/s^2$
M^L	lift force	$kg\ m/s^2$
M^{LUB}	wall lubrication force	$kg\ m/s^2$
M^{VM}	virtual mass force	$kg\ m/s^2$
M^{TD}	turbulence dispersion force	$kg\ m/s^2$
$\dot{m}$	mass flow rate	kg /s
N	extensive property	-
P	pressure	kg/ms^2

P_k	shear production of turbulence	kg/ms^3
P_{tot}	total pressure	kg/ms^2
R	gas constant	m^{3}Pa /K mol
r_α	volume fraction of phase α	-
S_M	momentum sources due to external body forces	kg/m^{2}s^2
S_{MS}	mass sources	kg/m^{3}s
t	time	s
U, u	velocity	m/s
V	volume	m^3
v	kinematic viscosity	m^2/s
X	mole fraction	-
x, y, z	Cartesian coordinates	-
Y	mass fraction	-

Greek Symbols

Symbol	Description	Dimensions
ϵ	turbulence eddy dissipation	m^2/s^3
ϵ_g	gas hold-up	-
η	intensive property	
Γ	mass flow rate per unit volume	kg/m^{3}s
κ	turbulence kinetic energy	m^2/s^2
μ	viscosity	kg/ms
ρ	density	kg/m^3
σ	schmidt number	-
τ	mean residence time	s
τ	shear stress	kg/ms^2

Subscripts

α	phase α in mixture
β	phase β in mixture
c	continuous phase
d	dispersed phase
eff	effective
g	gas
ip	integration point
i, j	unit vectors in coordinate directions
L	liquid
P	particle
R	reactor
t	turbulence
W	wall
z	axial coordinate

Dimensionless numbers

Bo	Bodenstein number
Eo	Eotvos number
M	Morton number
Re	Reynolds number
Sc	Schmidt number
St	Stanton number

Contents