

**MODELING AND SIMULATION STUDIES ON GAS  
ABSORPTION IN A CONTINUOUS FILM  
CONTACTOR**

by

**AKANKSHA**

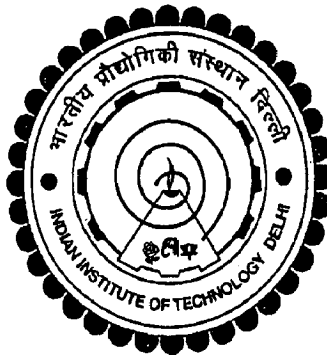
**DEPARTMENT OF CHEMICAL ENGINEERING**

*Submitted in fulfillment of*

*the requirements of the degree of*

**DOCTOR OF PHILOSOPHY**

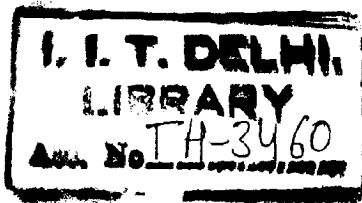
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*PARENTS*

## CERTIFICATE

This is to certify that the thesis entitled, “**MODELING AND SIMULATION STUDIES ON GAS ABSORPTION IN A CONTINUOUS FILM CONTACTOR**” being submitted by **Ms. Akanksha** to the Indian Institute of Technology, Delhi for the award of Doctor of Philosophy is a record of bonafide research work carried out by her under our guidance and supervision in conformity with the rules and regulations of Indian Institute of Technology Delhi.

The research report and results presented in this thesis have not been submitted, in part or full, to any other university or institute for the award of any degree or diploma.


  
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## ACKNOWLEDGEMENT

*First of all, I would like to thank my advisor Prof. V. K. Srivastava, Professor, Department of Chemical Engineering, for his constant support and supervision in the Ph.D. program. Dr. Srivastava showed great interest in my development as a researcher and I learned a lot from our numerous weekly meetings. He encouraged questions and always tried to inspire independent thoughts. He showed me different ways to approach the research problem and the need to be persistent to accomplish any goal. The keen interest shown by him with unflinching patience and indefatigability has been a source of inspiration to me and has enabled me to bring this work to a successful completion, which may not otherwise have been possible.*

*I am extremely grateful to my co-supervisor, Dr. K. K. Pant, Associate Professor, Department of Chemical Engineering, who is most responsible for helping me complete the writing of this dissertation as well as the challenging research that lies behind it. Dr. Pant has been a friend and mentor. He taught me how to write academic papers, made me a better programmer, had confidence in me when I doubted myself, and brought out the good ideas in me. Without his encouragement and constant guidance, I could not have finished this dissertation. He was always there to meet and talk about my ideas, to proofread and mark up my papers and chapters, and to ask me good questions to help me think through my problems. His keen faith, sincere*

*encouragements, and zealous interest in every aspect of my work are wholeheartedly acknowledged.*

*I am highly indebted to both of my supervisors for inculcating within me the qualities of perseverance, confidence and a sense of commitment towards one's work. It was a fortunate and unforgettable experience to work under their reflective and revered guidance. Their endless kindness and incomparable support cannot be thanked adequately here.*

*I am profoundly thankful to Prof S. K. Gupta, Head, Chemical Engineering Department, for providing me with all the necessary facilities during the course of my work.*

*I would also like to express my gratitude to my thesis committee, Prof. G. P. Aggrwal, Prof. K. D. P. Nigam and Prof. A. K. Gupta for their encouragement, constant support, necessary suggestions and for asking me good questions and rescuing me from various red tape crisis.*

*I wish to convey my sincere thanks to Prof. A.K. Gupta for some fruitful discussions and invaluable suggestions during the compilation of my experimental work. Special thanks to Dr. P. M. Pandey, Department of Mechanical Engineering, for his valuable contributions in successful inclusion of the optimization studies in my research work.*

*The encouragement, constant support, critical reviews and important suggestions given by Dr. A. N. Bhaskarwar, Prof. B. K. Guha, Prof. D.Subbarao, Dr. S. Roy and Prof. T. R. Rao during the departmental*

*seminar sessions are greatly acknowledged. I also wish to thank the other faculty members and office staff of the Department.*

*Nothing can be done without proper environment for the research work to be carried out. In this regard I should not forget to acknowledge the people for providing me excellent work environment in the laboratory, which facilitated my research to a great deal. I thank Mr. N. K. Gupta, lab-in-charge, Mr. D. K. Gupta, Mr. Krishna Kumar and Mr. Badri Prasad for their constant help in every possible way. I am also thankful to Mr. Inderjeet Singh, Mr. Rajinder Khanna, Mr. Nayak, Mr. Vijay Pal, Mr. Selva Ganapathi, Mr. Ashwani Kumar and Mr. Ramesh for their help and assistance rendered during the different stages of the experimental work. I am also grateful to the past and present members of the Laboratory of Chemical Reaction Engineering, Nandini, Sanjay Patel, Dr. Sapna Jain, Dr. Preeti Sahai, Dr. Tony, Dr. Hasan, Vikrant Sarin for their help and the friendly scientific and social environment.*

*I would also like to gratefully acknowledge the support of some very special individuals. Vimal deserves a special mention here for providing me endless support in carrying out CFD studies. His unconditional support and lively companionship made my research work a really enjoyable experience. His cooperation, concern and encouragement in his own little ways actually pulled me through the tougher and tiring times. Vimal was a great facilitator. A very special thanks to my brother Kanthi for his continuous support and for reminding me that there is life beyond numerical modeling. I would also like to*

*acknowledge Rajeev Garg for being open, most of the time, to answer any questions regarding my research work.*

*Thanks are also due to Rekha Rattan, Sukhdeep Kaur, Navdeep, Papiya, Monisha, Subhashini, Arnab, Muthukrishnan, Senthilmurugan, Balamurugan, Narendra, Anand Singh, Ajit and other students for their kind concern and support. When one owes so many, it is almost impossible and invidious to single out names. However I acknowledge my well wishers and friends Mrs. Srivastava, Dr. Hema Pant, Arpita and Prashant for inspiring me throughout my Ph. D. work.*

*Last, but not least, I thank my family: my parents, for giving me life in the first place, for unconditional support and encouragement to pursue my interests, even when the interests went beyond boundaries of language, field and geography. I am also thankful to my sister Teena, and brother, Kunal for listening to my complaints and frustrations, and for believing in me.*

*Herewith I would like to thank all of those, who have directly or indirectly contributed to the realization of this thesis.*

*Finally, and most importantly, a note of heart felt devotion to GOD, who has made me capable of accomplishing this uphill task.*

*Akanksha*  
(AKANKSHA)

## ABSTRACT

Absorption process is widely used in large process installations, however, its only recently that substantial progress has been made in developing a fundamental understanding of these processes. Gas liquid absorption can be extremely complex due to the existence of a deformable interface with varying shapes and motion, transient and multidimensional behavior, flow instabilities and turbulence, a very complex combination of process thermodynamics and kinetics, with intricate reaction schemes and complex mass transfer-reaction coupling. Actual modeling of such systems will contribute substantially in designing and better understanding of the performance of the process and selecting the optimum process parameters which is likely to be valuable in the actual operation of industrial continuous film contactors (CFC). CFC's find applications in various industrial processes like absorption, crystallization, evaporation, boiling, distillation, coating and solar photochemical processes due to their simple and effective means of enhancement in heat and mass transfer, better control of flow rates and ease of construction.

The present research is mainly focused on carrying out modeling and simulation studies on gas liquid absorption for different reactive systems in a continuous film contactor. A steady state two-dimensional model has been developed to simulate the process of gas absorption inside a CFC. The proposed model couples the chemical interactions to convection and diffusion of liquid species in all the directions resulting in highly coupled partial differential equation of second order and ordinary differential equations of first order. The governing equations of mass, momentum and energy have been numerically solved with a backward implicit finite difference method and trapezoidal implicit scheme. The performance of the

numerical model has been validated with the experimental data of a detergent industry. The model is able to predict the behaviour of industrial scale film reactor with a reasonable degree of accuracy.

The applicability of the model has been further examined for the chlorination of n-decane. The chemical system is found to be highly sensitive and optimization studies have been carried out for parameter estimation using Genetic Algorithm (GA) technique. The results are found to be in good agreement with the published literature.

In another study, the absorption characteristics of CO<sub>2</sub> removal have been investigated both experimentally and numerically. An experimental test facility has been designed and commissioned in order to study the absorption of the CO<sub>2</sub> in aqueous monoethanolamine (MEA) solution flowing in the counter current fashion. Effect of gas and liquid flow rates, MEA concentration and CO<sub>2</sub> partial pressure has been studied. The mass transfer coefficient has been estimated and correlated based on the experimental results. It is observed that rate of absorption is strongly dependent on gas and liquid flow rates and other hydrodynamic conditions in the reactor.

In order to explore the flow physics of the targeted annular flow, a two dimensional model using computational fluid dynamics (CFD), volume of fluid (VOF) approach have been solved under the present experimental laminar flow conditions. The model gives a qualitative view of falling liquid film and is able to capture the important aspects of the flow patterns

throughout the entire contactor. The results show a wavy interface for very low liquid and gas Reynolds number, however the waves observed are of very low amplitudes.

The proposed numerical model has been finally modified according to the CO<sub>2</sub>-MEA experimental system. The governing transport equations based on momentum, mass and heat balance provides a mechanistic interpretation of the experimental results and a means to predict the gas absorption performance at arbitrary adjustments of operational parameters such as reactants (gas and liquid) concentration, flow rate of the absorbent, and flow rate of the gas mixture. The numerical predictions are in good agreement with the present experimental data.

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