

# **CFD STUDIES ON TRICKLE BED REACTORS**

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**DEPARTMENT OF CHEMICAL ENGINEERING**

**INDIAN INSTITUTE OF TECHNOLOGY DELHI**

**JULY 2009**

# **CFD STUDIES ON TRICKLE BED REACTORS**

by

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**DEPARTMENT OF CHEMICAL ENGINEERING**

*Submitted*

*in fulfillment of the requirements of the degree of*

**DOCTOR OF PHILOSOPHY**

*to the*



**INDIAN INSTITUTE OF TECHNOLOGY DELHI**

**JULY 2009**

## **CERTIFICATE**

This is to certify that the thesis entitled, '**CFD Studies on Trickle Bed Reactors**' being submitted by **Mr. Arnab Atta** to the Indian Institute of Technology Delhi for the award of Doctor of Philosophy is a record of bonafide research work carried out by him under my 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.

**(K. D. P. Nigam)**

Professor

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**Dedicated**  
**To**  
**My Beloved Parents**

**Ring the bells that still can ring**

**Forget your perfect offering.**

**There is a crack in everything,**

**That's how the light gets in.**

**~ Leonard Cohen**

*Canadian artist (1934 - )*

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**(Arnab Atta)**

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## Abstract

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Trickle bed reactors (TBRs) are multiphase reactors in which gas and liquid phases flow co-currently downward over a solid catalyst packing. TBRs find widespread use in petroleum refining, chemical and process industries, pollution abatement and biochemical industries. The design and scale up of TBRs which depend on key hydrodynamic variables such as liquid volume fraction (liquid saturation), particle-scale wetting and overall gas–liquid distribution, continues to be a major challenge for chemical engineers. These variables are difficult to determine experimentally and interactions between these are poorly understood so far. Even though numerous experimental studies have been reported on measurement of these variables, predicting them from first principle hydrodynamic simulations is not an easy task and no coherent as well as conclusive methodology for doing so has yet been espoused.

Increasing computational power and development of computational fluid dynamics (CFD) has allowed promising applications of numerical simulations to the modeling of multiphase flow in TBR. While the CFD models have tried to resolve the existing complexities of the TBR to a great extent, considerable debate still persists on the exact nature of equations to be solved for TBR simulations. Depending on the problem formulation and requirement of specific results, some of the open issues include the number of phases to be solved, the nature of the model (steady state or transient), the formulation of the equations (Euler–Euler or Euler–Lagrange), the level of details in describing the packed bed (i.e., the particle-scale models) and, the appropriate boundary and initial conditions to be used. Most of the literature available dealing with

packed bed flow simulations uses a three-phase Eulerian model in which the solid velocity is identically set to zero. Such a calculation is nevertheless computationally demanding and yet experiments have not advanced to a level (except perhaps the MRI imaging studies) wherein the flow features predicted at the particle and liquid-rivulet scale in the TBR can be captured with fidelity. Even in the MRI studies, which can be indeed intriguingly sophisticated, only aid in high resolution flow visualization but a one-to-one comparison with the CFD computation is not possible. That being the present scenario, and the fact that even the multi-fluid CFD models have a lot of questionable assumptions (even though deceptively at a micro-scale), the wisdom of using a highly computationally intensive model for predicting global profiles in a TBR may be questioned. In light of that, in this dissertation, a less computationally intensive, yet first-principle based CFD model has been presented using the porous media concept.

A comprehensive CFD based model has been developed for predicting hydrodynamic parameters in trickle bed reactors under cold-flow conditions. The two-phase Eulerian model describing the flow domain as a porous region has been used to simulate the macroscale multiphase flow in trickle beds operating under trickle flow regime using a commercial CFD solver. The closure terms for phase interactions has been addressed by adopting the relative permeability concept. The model has been evaluated by comparing predictions with the data (collected under a varied set of laboratory conditions) available in the open literature. It is shown that while being relatively simple in structure, this CFD model is flexible and predictive for a large body of experimental data presented in the open literature.

Thereafter it is extended to a three-dimensional CFD model to understand and forecast the liquid maldistribution in TBRs under cold-flow conditions. The model predictions are validated against experimental data reported in literature. Various distributor configurations have been tested in the CFD model and sensitivity studies have been performed. Good agreement is obtained between the reported experimental results and the proposed first-principle based CFD model. The concept of distribution uniformity is then discussed and applied to the CFD model predictions. The CFD model is subjected to a systematic sensitivity study in order to explore better liquid distribution alternatives.

Since, most commercial TBRs employed in hydroprocessing and other industrially relevant operations normally operate at elevated pressures, an effort has been made to assess the complex hydrodynamics of high-pressure TBR using the developed CFD model. Different combinations of relative permeability correlations in the closure terms have been exercised to predict pressure drop and liquid saturation and to realize the *best fit*. The comparisons between model predictions and numerous experimental data, collected from different independent sources under varied set of operating conditions, lead to the favourable implementation of this less computationally intensive, yet first-principle based CFD model to forecast the two-phase hydrodynamics for high-pressure TBRs.

Cyclic operation as a potential measure for process intensification of TBR has gained substantial interests amongst the professionals. Despite its known advantages, scale up and applicability in commercial processes is still far from reality. To understand the transport processes and to analyze the inherent flow dynamics during wave propagation

in a cyclic TBR, the study has also been focused on a solitary square-wave liquid feed to visualize its behavior, effect and attenuation in the bed. Experiments for multiphase flow visualization and local variable measurement using electrical capacitance tomography (ECT) were carried out to follow the solitary liquid-rich wave in the bed. The developed two-phase Eulerian framework has been successfully applied for CFD modeling of different cyclic operation strategies in trickle bed reactors. The results assert the efficacy of slow mode operation since the wave attempts to preserve its identity while propagating in the bed. The decay time in case of fast mode cyclic operation is prolonged and continues to attenuate down the reactor length. The predictive computational model used in this work, in spite of many simplifications, conforms arguably well with the experimental observations.

Since, TBRs are regularly utilized in all petroleum refining industries, it is expected that any optimistic contribution towards its design and/or modeling of different parameters will not only lead to technology development but will also help to sustain a cleaner and greener environment.

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# Table of Contents

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<b>Certificate</b>	<i>i</i>
<b>Acknowledgement</b>	<i>iv</i>
<b>Abstract</b>	<i>vii</i>
<b>Table of Contents</b>	<i>xi</i>
<b>List of Figures</b>	<i>xiv</i>
<b>List of Tables</b>	<i>xix</i>
<b>Chapter 1: General Introduction</b>	<b>1</b>
1.1. Trickle bed reactors	1
1.1.1. Flow regime	2
1.1.2. Pressure drop and liquid holdup	3
1.1.3. Liquid maldistribution	6
1.1.4. High pressure operation	10
1.1.5. Periodic operation	11
1.2. Computational fluid dynamics (CFD) modeling	13
1.3. Scope and objectives	16
1.4. Outline of the dissertation	18
Notation	19
Literature cited	20
<b>Chapter 2: CFD Modeling of Pressure Drop and Liquid Holdup</b>	<b>26</b>
2.1. Introduction	27
2.2. Scope and objective	29
2.3. Model development	29

2.3.1.	Governing equations of the flow	31
2.3.2.	Relative permeability model	32
2.4.	Model setup and numerical solution procedure	36
2.5.	Results and discussion	38
2.6.	Conclusions	46
	Notation	48
	Literature cited	49
<b>Chapter 3:</b>	<b>Investigation of Liquid Maldistribution</b>	<b>54</b>
3.1.	Introduction	55
3.2.	Scope and objective	58
3.3.	Governing equations of the flow	58
3.4.	Model setup and numerical solution procedure	60
3.5.	Results and discussion	66
3.6.	Conclusions	76
	Notation	78
	Literature cited	80
<b>Chapter 4:</b>	<b>High Pressure Operation : Effect of Relative Phase Permeabilities</b>	<b>84</b>
4.1.	Introduction	85
4.2.	Scope and objective	88
4.3.	Model equations	89
4.4.	Model setup and numerical solution procedure	93
4.5.	Results and discussion	95
4.6.	Conclusions	112

Notation	113
Literature cited	114
<b>Chapter 5: Liquid Feed Cycling in Trickle Bed Reactors</b>	<b>118</b>
5.1. Introduction	119
5.2. Scope and objective	121
5.3. ECT setup and experimental procedure	122
5.4. Relevance of the systematic experimental observation	124
5.5. Numerical modeling of solitary square-wave liquid feed	129
5.5.1. Governing equations	129
5.5.2. Model setup and solution procedure	131
5.5.3. Results and discussion	132
5.6. Conclusions	135
Notation	136
Literature cited	137
<b>Chapter 6: Concluding Remarks and Future Recommendations</b>	<b>140</b>
6.1. Summary of conclusions	140
6.2. Recommendations of future work	143
<b>Appendix A Representative Photographs of ECT</b>	<b>145</b>
<b>Author's Bio-data</b>	<b>147</b>