CHEMICAL REACTORS

H. Scott Fogler, Editor

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Chemical Reactors

H. Scott Fogler, EDITOR
The University of Michigan

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sponsored by the Division of
Industrial and Engineering Chemistry
at the Second Chemical Congress
of the North American Continent
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FOREWORD

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PREFACE

The symposium upon which this volume is based focused on three areas in reaction engineering: fluidized bed reactors, bubble column reactors, and packed bed reactors. Each area comprises a section of this book. Professor J. R. Grace chaired and coordinated the fluidized bed sessions; Professors Y. T. Shah and A. Bishop, the bubble column reactor session; and Professor A. Varma, the packed bed reactor session. Each section in this book opens with a brief review chapter by the session chairman that includes an overview of the chapters in each session.

Fluidized bed reactors have received increased interest in recent years owing to their application in coal gasification. The section on fluidized beds discusses critical areas in fluid bed reactor modeling. Computer simulation of both solid-catalyzed gas phase reactions as well as gas–solid reactions are included.

In the section on bubble column reactors, the hydrodynamic parameters needed for scale-up are presented along with models for reaction and heat transfer. The mixing characteristics of columns are described as are the directions for future research work on bubble column reactors.

The packed bed reactors section of this volume presents topics of catalyst deactivation and radial flow reactors, along with numerical techniques for solving the differential mass and energy balances in packed bed reactors. The advantages and limitations of various models (e.g., pseudo-homogeneous vs. heterogeneous) used to describe packed bed reactors are also presented in this section.

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FLUIDIZED BED REACTORS

Fluidized Bed Reactor Modeling

An Overview

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Critical areas in fluid bed reactor modeling are discussed in the light of papers in this symposium. There continues to be a wide diversity of assumptions underlying models. However, it is now clear that predictions are generally much more sensitive to some assumptions than to others. For example, proper modeling of interphase exchange is generally more critical than the assumptions adopted to describe axial gas dispersion in the dense or emulsion phase. For the 1980's advances are looked for in a number of areas, especially in more sophisticated computer models, unsteady state representations suitable for control purposes, models which describe high velocity regimes of fluidization, inclusion of grid and freeboard effects, and study of radial gradients.

This volume brings together a number of papers under the theme of fluidized bed reactor modeling. This field is of relatively recent origin. Table I gives the emphasis in research in successive decades beginning with the 1940's. It is seen that early research was devoted primarily to practical problems associated with the operation of fluidized bed reactors and to very simple models. With the passage of time models have been devised which are increasingly sophisticated. Reviews of the commercial development of fluidized beds as reactors have been prepared by Geldart (1,2). In the 1970's there were a number of reviews (3-7) which considered fluidized bed reactor modeling.

In order to be able to represent the behaviour of fluidized bed reactors with confidence, one must have a thorough understanding of the bed hydrodynamics and of the reaction kinetics. Almost all of the reactions carried out in fluidized beds are either solid-catalysed gas phase reactions or gas-solid reactions. (We will not consider here homogeneous gas phase reactions, reactions in liquid fluidized beds or reactions in three phase fluidized beds.) While the chemical kinetics can often be highly complex,

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for example in the gasification or combustion of coal, the hydrodynamic aspects have given the greatest difficulty and have been subject to the greatest debate. While considerable progress has been made in achieving an understanding of many aspects of bed behaviour, there are many features which remain poorly understood. Some of these (e.g. regimes of bed behaviour, gas mixing patterns, and exchange of gas between phases) can affect profoundly the nature of the model adopted.

Table I: Focus of Research on Fluidized Bed Reactors

Decade	Emphasis
1940's	Practical design and operation problems. Single phase models only.
1950's	Simple two-phase models for gas-phase solid-catalysed reactions.
1960's	Incorporation of properties of single bubbles. Early models for gas-solid reactions.
1970's	Addition of end (grid and freeboard) effects. More sophisticated models for specific gas-solid reactions including energy balances. Consideration of complex kinetics.
1980's	? Probable emphasis on non-bubbling (turbulent and fast fluidization) regimes. Probable consideration of effects of aids to fluidization (e.g. centrifugal, magnetic and electrical fields, baffles). Increasing emphasis on more complex hydrodynamics and kinetics, with models requiring computers for solution.

The papers presented at the Las Vegas symposium, most of which are reproduced in this volume, both illustrate the diversity of modeling approach and show some new directions for reactor modeling in the 1980's. Before turning to these matters in detail, it is necessary to discuss briefly three of the papers which are fundamentally different in focus from the other eight.

The paper by Ramírez *et al* (8) considers the important question of particle-to-gas heat transfer in fluidized beds. In addition to the importance of this question in its own right, particle-to-gas heat transfer can be important for fluid bed reactors, for example in determining thermal gradients in the entry (grid) region, in establishing the surface temperature of particles undergoing reactions, and via the analogous case of gas-to-particle mass transfer. There has been considerable controversy over the fact that Nusselt and Sherwood numbers have been found to fall well below 2, the lower limit for a single sphere in a stagnant medium. Ramírez *et al* produce further evidence of $Sh \ll 2$ and $Nu \ll 2$ and consider these results in the light of transfer models in the literature.

The paper by Blake and Chen (9) represents an extension of the novel approach adopted by the Systems, Science and Software group. In what must be the most ambitious and comprehensive fluidization modeling effort to date, this group has used modern computational techniques to solve a set of equations representing the physics and chemistry of fluidized bed coal gasifiers. Hydrodynamic fixtures are represented by a set of continuum equations and constitutive relationships, while chemical kinetics equations are written for key heterogeneous and homogeneous reactions based on studies reported in the literature. In previous papers, the authors have shown that the model gives a realistic simulation of a jet of gas issuing into a bed of solids. In the present paper they seek to duplicate results obtained in the IGT and Westinghouse pilot scale reactors. The results are of considerable interest, giving a good match with most of the experimental results.

A further paper by Gibbs (10) deals with design and modeling of centrifugal fluidized beds. In this case gas is fed radially inwards into a spinning bed. On account of the greatly augmented effective gravity force, greater through-puts of gas can be accommodated and entrainment is greatly lowered. This new technique has received attention in the late 1970's especially in connection with coal combustion. Some unique problems are encountered, e.g. the minimum fluidization velocity becomes a function of bed depth, while particles ejected into the "freeboard" by bubbles bursting at the bed surface travel initially nearly at right angles to the gas exit direction. This paper gives a preliminary scheme for dealing with some of these problems.

Classification of Reactor Models

There are many choices to be made in fluid bed reactor modeling and little unanimity among those who devise such models on the best choices. Table II lists some of the principal areas for decision and the corresponding choices of the other eight papers at this symposium (11-18).

Phases. Both two-phase and three-phase representations are widely used as shown schematically in Figure 1. In two-phase representations the dilute phase may represent bubbles alone, jets (in the grid region), or bubbles plus clouds. Three-phase representations generally use the scheme followed by Kunii and Levenspiel (19) whereby bubbles, clouds, and "emulsion" (i.e. that part of the non-bubble bed not included in the clouds) are each treated as separate regions. As shown in Table II, all of these possibilities are represented in the models adopted by the authors in this symposium. There appears, however, to be an increasing tendency to adopt three phase models, probably as a result of experimental results (20) which showed that the Kunii and Levenspiel model gave a better representation of measured concen-

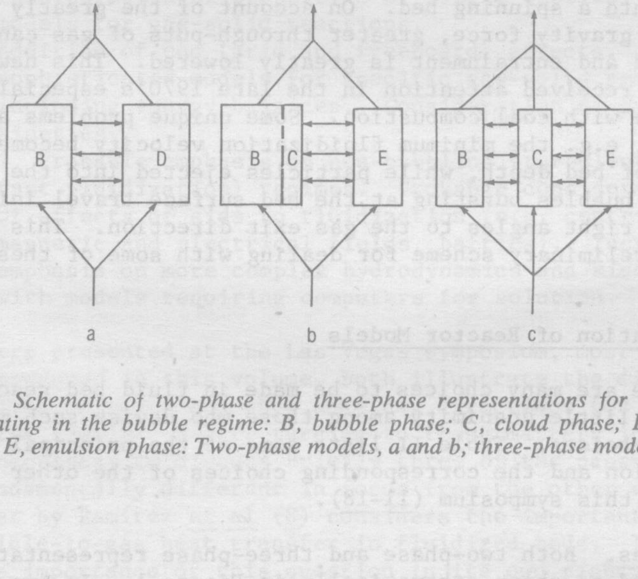

Figure 1. Schematic of two-phase and three-phase representations for fluidized beds operating in the bubble regime: B, bubble phase; C, cloud phase; D, dense phase; E, emulsion phase: Two-phase models, a and b; three-phase models, c

tration profiles for a particular particle size than other models tested. The bubbles themselves are usually treated as being completely devoid of particles, but it is important (21) that solids dispersed in the bubbles be included with the bubble phase for fast reactions, even though their concentration is small (typically < 1% by volume).

Gas Mixing in the Dense or Emulsion Phase. No other feature of fluidized bed reactor modeling has been subjected to so many alternative assumptions as axial mixing in the dense phase. At least eight possibilities have been tried as shown in Figure 2. These range from upward plug flow, through perfect mixing and stagnant gas, to downflow. Intermediate degrees of mixing have been represented by axial dispersion models and well-mixed stages in series. As shown in Tabe II many of these possibilities have been covered in the present symposium.

In view of the large number of disparate representations of dense phase axial mixing, one might easily conclude that this is one of the more important modeling features. In practice this is not the case, unless high conversions (e.g. 90% or greater in a single stage) are sought. For lower conversions, overall reactor performance tends to be insensitive to the pattern of axial mixing adopted (21). There are several illustrations of this point in this symposium. In the paper by Jayaraman et al (16), replacement of the downflow condition adopted by Fryer and Potter (22) by perfect mixing in the emulsion led to conversions which were barely distinguishable from those given by the earlier model. (At the same time solution became much simpler.) Jaffres et al (15) show that the two extreme cases of perfect mixing and plug flow in the Orcutt models (23) lead to similar results. (In their case, however, bubble properties were varied together with kinetic constants in their optimization so it is harder to distinguish the influence of the mixing assumptions alone.) Elnashaie and Elshishini (12) further show that the effect of axial dispersion is not only relatively slight in terms of overall conversion, but that dense phase mixing also plays a relatively minor role in determining selectivity for consecutive reactions and multiplicity of steady states.

In almost all previous modeling work, one-dimensional flow has been assumed in each phase, radial gradients being taken as negligible. There is some experimental evidence (24) that substantial radial gradients may exist, however. Radial gradients are especially important for fluid bed combustors with in-bed feeding of fresh coal via a series of nozzles. In this case the rapid devolatilization reactions will occur close to the distributed feed points, and radial dispersion of volatiles away from these points and oxygen towards them will be extremely important if the volatiles are to burn out within the bed. Fan and Chang (13) have considered this problem, coupling an assumption of perfect axial mixing with a diffusion-type mixing model in the ra-

Table II: Key features of models used in this symposium

	de Lasa *et al* (11)	Elnashaie & Elshishini (12)	Fan & Chang (13)	Fogler & Brown (14)
Phases	2: Bubble (or jet) & dense or 1: (CSTR)	2: Bub/Cloud & emulsion or 3: Bubble, cloud & emulsion	2: Bubble & dense	3: Bubble, cloud and emulsion
Gas mixing in dense or emulsion phase	perfect mixing	perfect mixing or plug flow upward	perfect axial mixing + radial dispersion	stagnant
Interphase transfer	jet/dense: Behie (43) bub/dense: (27) or (19)	(37) or (19)	K-L (19)	K-L (19)
Distribution of flow between phases	Two phase theory	2-ϕ theory + cloud or $U_{mf}A_{emulsion}$ through	Two phase theory	Two phase theory
Bubble size	Basov equation (constant)	Kept as parameter (constant)	Kept as parameter (constant)	Mori & Wen (varies)
Heat balance?	Yes	Yes	Yes	No
Time variation	steady	steady	unsteady	steady
Reaction	gas-solid	catalytic	gas-solid	catalytic
Application	Catalyst regenerator	consecutive reactions	Coal combustion	general
Experimental data	large unit	none	none	none

Table II: Key features of models used in this symposium (Continued)

	Jaffres et al (15)	Jayaraman et al (16)	Peters et al (17)	Rehmat et al (18)
Phases	2: Bubble & dense	3: Bubble, cloud & emulsion	3: Bubble, cloud & emulsion	3: Gas, char & limestone
Gas mixing in dense or emulsion phase	plug flow or perfect mixing	perfect mixing	compartments in series	all gas in plug flow upward
Interphase transfer	D-H (27)	K-L (19)	K-L (19)	N.A.
Distribution of flow between phases	Two phase theory	as Fryer and Potter	New approach	N.A.
Bubble size	Mori & Wen & fitted values (constant)	specified value (constant)	Mori & Wen (varies)	N.A.
Heat balance?	Yes	No	No	Yes
Time variation	unsteady	steady	steady	steady
Reaction	catalytic	catalytic	pseudo-catalytic	gas-solid
Application	Maleic anhydride	general	Aerosol filtration	Coal combustion
Experimental data	cf. earlier data	none	cf. earlier data	none

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