01 Jan 2000

Discriminating Trickle-Flow Hydrodynamic Models: Some Recommendations

F. Larachi

I. Iliuta

M. (Muthanna) H. Al-Dahhan
Missouri University of Science and Technology, aldahhanm@mst.edu

M. P. Dudukovic

Recommended Citation

F. Larachi et al., "Discriminating Trickle-Flow Hydrodynamic Models: Some Recommendations," *Industrial and Engineering Chemistry Research*, vol. 39, no. 2, pp. 554 - 556, American Chemical Society, Jan 2000.
The definitive version is available at https://doi.org/10.1021/ie990632y

Discriminating Trickle-Flow Hydrodynamic Models: Some Recommendations

F. Larachi,*,† I. Iliuta,‡ M. A. Al-Dahhan,§ and M. P. Dudukovic§

Department of Chemical Engineering & CERPIC, Laval University, Québec, Canada G1K 7P4, Department of Chemical Engineering, Faculty of Industrial Chemistry, University Politehnica of Bucharest, Polizu 1, 78126 Bucharest, Romania, and Chemical Reaction Engineering Laboratory (CREL), Washington University, St. Louis, Missouri 63130

The forecasting ability of five one-dimensional (1-D) two-fluid phenomenological models for liquid holdup and two-phase pressure drop in trickle-flow reactors was evaluated using the most comprehensive trickle-flow regime database. All of these models, namely, the permeability model, the slit model, the extended slit model, the 1-D CFD model, and the double-slit model can be used to predict liquid holdup. Among them, the permeability and the slit models, because of a much simpler structure, are recommended. The extended slit model based on Iliuta et al. (*Ind. Eng. Chem. Res.* **1998**, *37*, 4542) shear and slip constitutive relationships can be employed for two-phase pressure drop predictions. When the knowledge of wetting efficiency becomes essential at very low liquid flow rates, the double-slit model is recommended.

1. Introduction

Trickle-bed reactors have achieved widespread acceptance in various three-phase catalytic commercial applications. They are employed in the petroleum and petrochemical and chemical industries in the destruction of aqueous biocidal compounds, in bio- and electrochemical processing.[1,2] Though they are the focus of intense academic research over almost half a century,[3] proper design of trickle beds, despite their industrial relevance, continues to rely by and large on know-how. Despite a formidable amount of work related to the study of trickle-bed hydrodynamics, no consensus has emerged as to whether general approaches yielding pressure drop and liquid holdup with acceptable accuracy can be recommended. This is ascribable to many causes, among which the following are most frequently mentioned:

(i) The complexity of the gas−liquid flow patterns prevailing in trickle beds.

(ii) The lack of accurate descriptors of two-phase flow interactions.

(iii) The complex relationship between trickle-bed hydrodynamic characteristics, fluids and bed properties, and interfacial interactions.

(iv) The restricted range of the experimental data, and of the models/correlations derived thereof, usually reported for individual studies.

All of the above results in design tools unable to describe and quantify adequately the relevant hydrodynamic phenomena observed in trickle-bed reactors.

Since the pioneering studies of the 1950s,[4] it is estimated that approximately 30 000 experimental data on co-current packed-bed reactor hydrodynamics were released worldwide in the open literature. Beyond half of them were for two-phase pressure drop and liquid holdup in trickle beds. An advanced database, covering broad ranges of fluid properties, operating conditions, and bed characteristics, is being set[4] based on this accessible literature information to provide a frame basis for meticulous analysis and systematic comparisons with the ultimate goal of recommending the best estimation tools for trickle-bed hydrodynamic characteristics. The gathered abundant experimental data is largely diversified and continually expanded and updated, making the information both useful and more practical in verification of research ideas. About 4 000 experiments from this database were carried out deep in the trickle-flow regime and encompassed full wetting as well as partial wetting conditions. This flow regime usually occurs at low liquid and gas throughputs and represents an industrially relevant contacting pattern.

The aim of this short communication is to test some recent models for liquid holdup and pressure drop for the *trickle-flow regime* against the largest database ever collected using most of the hydrodynamic information available since 1959. Although these models use different premises,[5−8] they can all be formally recasted into the familiar unidirectional segregated two-fluid model possessing both creeping and inertial flow terms. The variations among these models arise from assumptions such as the following:

(i) Interaction-free gas−liquid interface impervious to momentum transfer.[5,6,9]

(ii) Momentum active gas−liquid interface with mutual phase interactions.[7,10,11]

(iii) Momentum active gas−liquid interface with mutual phase interactions, wetting efficiency, and gas−solid drag in a partially wetted trickle-flow regime.[8]

The following 1-D segregated two-fluid models ("permeability" model,[5] slit model,[6,9] extended slit model,[10,11] "1-D CFD" model,[7] double-slit model[8]) emerged, so far, as being the best frameworks designed for the description of trickle-flow hydrodynamics. They are thus confronted with the database content and then discrimi-

* To whom correspondence should be addressed. Tel.: 1-418-656-3566. Fax: 1-418-656-5993. E-mail: flarachi@gch.ulaval.ca.
† Laval University.
‡ University Politehnica of Bucharest.
§ Washington University.

10.1021/ie990632y CCC: $19.00
Published on Web 12/21/1999

Table 1. Statistical Tests of Models/Correlations for Liquid Holdup and Two-Phase Pressure Drop in Trickle-Flow Regime

	statistical parameter							
	trickle flow, all data				trickle flow, partial wetting data			
	$\langle e_Y \rangle$ (%)		σ (%)		$\langle e_Y \rangle$ (%)		σ (%)	
reference	$\Delta P/H$	ϵ_L	$\Delta P/H$	ϵ_L	$\Delta P/H$	ϵ_L	$\Delta P/H$	ϵ_L
Models								
Saez and Carbonell[5]	53	19	56	48	46	26	26	82
Holub et al.[6,9]	74[a]	15[a]	19	14	69	21	25	19
Holub et al.[6,9]	70[b]	18[b]	22	15				
Al-Dahhan et al.[10]	68[c]	13[c]	22	13				
Iliuta et al.[11]	35[d]	12[d]	26	11	41	25	22	16
Iliuta et al.[8]					32	24	23	29
	62[e]	20[e]	48	17	57[e]	25[e]	46	31
Attou et al.[7]	61[f]	20[f]	45	18	58[f]	23[f]	48	17
	65[g]	19[g]	45	18				
Empirical Correlations								
Ellman et al.[12,13]	70	25	27	30				
Larachi et al.[14]	72	20	33	22				

[a] E_1 and E_2 determined from single-phase flow experiments. [b] $E_1 = 180$ and $E_2 = 1.8$. [c] Extended Holub model, shear/velocity slip correlations from ref 10. [d] Extended Holub model, shear/velocity slip correlations from ref 11. [e] Original model (4 ODEs): accounts for pressure and holdup axial variation in bed. [f] Simplified model (2 ODEs): neglects holdup axial variation in bed. [g] Original model (4 ODEs): (E_1, E_2) correlation of Iliuta et al.[11] instead of 180, 1.8.

nated using the mean relative error between the predicted and experimental values,

$$\langle e_Y \rangle = \frac{100}{N} \sum_1^N \left| \frac{Y_{\mathrm{exp},i} - Y_{\mathrm{calc},i}}{Y_{\mathrm{exp},i}} \right| \qquad (1)$$

and the deviation of the relative error around the mean relative error,

$$\sigma = 100 \times \sqrt{\frac{1}{N-1} \sum_1^N \left(\left| \frac{Y_{\mathrm{exp},i} - Y_{\mathrm{calc},i}}{Y_{\mathrm{exp},i}} \right| - \langle e_Y \rangle \right)^2} \qquad (2)$$

where Y in eqs 1 and 2 stands for the pressure drop or the liquid holdup.

2. Recommendations

For the sake of brevity, the reader is directed to ref 11 where the trickle-flow database is described in detail. Comparison of the models was achieved first using the complete database containing the cases of partial wetting as well as complete wetting of particles. Then, the data that fulfilled the partial wetting condition were extracted and compared separately to the same models. Hence, only the experiments carried out far remote and down of the trickle-to-pulse flow regime boundary were selected, that is, ca. 1200 pieces of data. For this purpose, a rule-of-thumb criterion of a liquid superficial velocity at most equal to the fifth of the liquid transition velocity was chosen as a conservative upper limit.

The respective scatters between the experimental values of pressure drop/liquid holdup and their predictions by the different models are summarized in Table 1. Although many correlations exist in the literature, we compared to this database the predictions by the empirical correlations of Ellman et al.[12,13] and Larachi et al.[14] because these are the only ones based on broad data sets. These correlations predicted pressure drop with a mean error of 70% and holdup with a mean error of 20%.

Irrespective whether data for the partially wetted beds only or for the whole trickle-flow regime was considered, the slit model[6,9] predicted well the liquid holdups but its performance at forecasting pressure drops was as weak as that by the above empirical correlations. Whether the genuine experimentally determined Ergun bed constants or the admittedly used estimates are used seems not to significantly affect the model predictions.

Also included in Table 1 are comparisons by the "extended slit" model,[10,11] the "permeability" model,[5] the "1-D CFD" model,[7] and the "double-slit" model.[8]

The "1-D CFD" model[7] and the "extended slit" model using Al-Dahhan et al.[10] constitutive shear and slip correlations did not improve much the pressure drop predictions. However, although of a much simpler structure, the "permeability" model[5] outperformed them on both whole trickle-flow data and partial wetting data as far as the mean error is concerned. The scatter around the mean error was however substantially higher. Moreover, the different simplifying assumptions under which the "1-D CFD" model[7] was tested appeared not to provide significant gains. It is suggested therefore to use this model in its simplest form, that is, by neglecting the stream-wise holdup variations (incompressible flow assumption, 2 ODEs) and by taking the Ergun constants recommended by Holub et al.[6] The "extended slit" model using Iliuta et al.[11] shear and slip constitutive relationships and the "double-slit" model[8] outperformed all the available models in terms of the pressure drop predictability whether the whole database or only the partial wetting conditions are considered. However, it was found that all six formulations performed almost equally well and can be recommended indistinguishably in liquid holdup predictions. In accordance with our previous observation,[10] these 1-D two-fluid models require a refined description of the interfacial interactions only for pressure drop. On the contrary, liquid holdup estimation in trickle flow does not require such a detailed interfacial description. Furthermore, except for the double-slit model, the inherent limitation of the other models lies in their inability to predict the wetting efficiency.

Literature Cited

(1) Meyers, R. A. *Handbook of Petroleum Refining Processes*, 2nd ed.; McGraw-Hill: New York, 1996.

(2) Dudukovic, M. P.; Larachi, F.; Mills, P. L. Multiphase Reactors—Revisited. *Chem. Eng. Sci.* **1999**, *54*, 1975.

(3) Larkins, R. P. Two-Phase Cocurrent Flow in Packed Beds. Ph.D. Dissertation. University of Michigan, Ann Arbor, MI, 1959.

(4) Iliuta, I.; Ortiz-Arroyo, A.; Larachi, F.; Grandjean, B. P. A.; Wild, G. Hydrodynamics and Mass Transfer in Trickle-Bed Reactors: An Overview. *Chem. Eng. Sci.* **1999**, *54*, 5329.

(5) Saez, A. E.; Carbonell, R. G. Hydrodynamic Parameters for Gas—Liquid Cocurrent Flow in Packed-Beds. *AIChE J.* **1985**, *31*, 52.

(6) Holub, R. A.; Dudukovic, M. P.; Ramachandran, P. A. A Phenomenological Model of Pressure Drop, Liquid Holdup and Flow Regime Transition in Gas—Liquid Trickle Flow. *Chem. Eng. Sci.* **1992**, *47*, 2343.

(7) Attou, A.; Boyer, C.; Ferschneider, G. Modelling of the Hydrodynamics of the Cocurrent Gas—Liquid Trickle Flow Through a Trickle-Bed Reactor. *Chem. Eng. Sci.* **1999**, *54*, 785.

(8) Iliuta, I.; Larachi, F.; Al-Dahhan, M. H. A Double-Slit Model for Partially Wetted Trickle Flow Hydrodynamics. *AIChE J.*, in press.

(9) Holub, R. A.; Dudukovic, M. P.; Ramachandran, P. A. Pressure Drop, Liquid Holdup and Flow Regime Transition in Trickle Flow. *AIChE J.* **1993**, *39*, 302.

(10) Al-Dahhan, M. H.; Khadilkar, M. R.; Wu, Y.; Dudukovic, M. P. Prediction of Pressure Drop and Liquid Holdup in High-Pressure Trickle-Bed Reactors. *Ind. Eng. Chem. Res.* **1998**, *37*, 793.

(11) Iliuta, I.; Larachi, F.; Grandjean, B. P. A. Pressure Drop and Liquid Holdup in Trickle Flow Reactors: Improved Ergun Constants and Slip Correlations for the Slit Model. *Ind. Eng. Chem. Res.* **1998**, *37*, 4542.

(12) Ellman, M. J.; Midoux, N.; Laurent, Charpentier, J. C. A New Improved Pressure Drop Correlation for Trickle-Bed Reactors. *Chem. Eng. Sci.* **1988**, *43*, 2201.

(13) Ellman, M. J.; Midoux, N.; Wild, G.; Laurent A.; Charpentier, J. C. A New Improved Liquid Holdup Correlation for Trickle-Bed Reactors. *Chem. Eng. Sci.* **1990**, *45*, 1667.

(14) Larachi, F.; Laurent, A.; Midoux, N.; Wild, G. Experimental Study of a Trickle-Bed Reactor at High Pressure: Two-Phase Pressure Drop and Liquid Saturation. *Chem. Eng. Sci.* **1991**, *46*, 1233.

Received for review August 20, 1999
Revised manuscript received November 11, 1999
Accepted November 11, 1999

IE990632Y