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Investigation of liquid maldistribution in trickle-bed reactors using porous media concept in CFD

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Abstract

A *three-dimensional* CFD model for simulating two-phase flow in trickle-bed reactors (TBRs) is presented. Based on porous media concept, a two-phase Eulerian model (rather than computationally demanding traditional three-phase Eulerian model) describing the flow domain as porous region is presented to understand and forecast the liquid maldistribution in TBRs under cold-flow conditions. The drag forces between phases have been accounted by employing the relative permeability concept [Sàez, A. E., Carbonell, R. G., 1985. Hydrodynamic parameters for gas–liquid cocurrent flow in packed beds. A.I.Ch.E. Journal 31, 52–62].

The model predictions are validated against experimental data reported in literature, notably using the liquid distribution studies of Marcendelli [1999. Hydrodynamique, Transfert de Chaleur Particule-Fluide et Distribution des phases dans les Reacteurs a lit Fixe a Ecoulement a Co-courant Descendant de Gaz et de Liquide. Doctoral Thesis. INPL, Nancy, France]. Various distributor configurations reported therein have been recreated in the CFD model and sensitivity studies have been performed. Good agreement is obtained between the reported experimental results and this proposed first-principle based CFD model.

Finally, the concept of distribution uniformity is 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.

Keywords: Trickle-bed; Porous media; Liquid distribution; CFD; two-phase flow

1. Introduction

Three-phase reactors (G-L-S) comprising a fixed bed of catalyst with flowing liquid and gaseous phases have various applications, particularly in the petroleum industry for hydroprocessing of oils (e.g. hydrotreating, hydrocracking). Trickle-bed reactors (TBR) are one of the most extensively used three-phase reactors. With a view towards developing more efficient TBR units in the future, for meeting stringent environmental and profitability targets, it is crucial that we develop the know-how for tailoring the flow patterns in them to optimally match the demands made by the kinetics of these reaction processes.

One of the critical issues in the efficient use of TBRs is the understanding and prediction of liquid maldistribution. With current interest in technologies of 'deep' processing, such as deep hydrodesulfurization, the need to be able to predict liquid maldistribution accurately is even more important, since small variations in liquid distribution can cause significant loss in activity in trickle-bed reactors operating close to 100% conversion (see for example, Harter et al., 2001). Regions of the TBR those are dosed by more than the required amount of liquid reactant and insufficient gas phase reactant may lead to under-utilization of the catalyst, while regions which have less than required amount of liquid may have both under-utilization of catalyst as well as formation of local hot spots (particularly in the case of highly exothermic reactions). Added to those are negative effects like coking of catalyst (particularly in petroleum refining applications), in regions of the TBR which are not exposed to the right amount of gas phase and liquid phase reactant. Liquid distribution also has a sharp impact on pressure drop, which may add significantly to the long-term operating cost of a TBR unit.

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Table 1
Recent investigation of liquid distribution in trickle-bed reactor

Investigator	Techniques of measurement	Experimental conditions	Observations/conclusion
Sapre et al. (1990)	Heater probe technique	Large scale commercial TBRs	(i) Maldistribution can occur above liquid mass flux of $4\,\mathrm{kg\,m^{-2}\,s^{-1}}$ (ii) Flow nonuniformity increase moving down the reactor
Lutran et al. (1991)	Computer assisted tomography	Square cross section (0.0603 m, l = 0.1905 m, d_p = 3–6 mm)	(i) Nonprewetted bed—filament flow (ii) Prewetted bed—film flow (iii) Large particle—film flow (iv) Low particle size—more pockets
Reinecke and Mewes (1996)	Capacitance tomography	$D_c = 120$ mm	(i) Increasing the liquid flow rate make the liquid distribution uniform (ii)Wall effect is more in small diameter column but is less in industrial columns
Saroha et al. (1998)	Liquid collector six zones	$l = 0.152$ m; Flow rate range $L = 1.46$–$7.31\,\mathrm{kg\,m^{-2}\,s^{-1}}$ $G = 0 - 0.043\,\mathrm{kg\,m^{-2}\,s^{-1}}$	(i) Increase in liquid or gas flow, improves the liquid distribution (ii) Decrease in liquid density and surface tension reduces the wall flow
Marcandelli et al. (2000)	Pressure drop measurement, RTD method, heat transfer sensor, capacitive tomography, and liquid collector nine zones.	$l = 1.3$ m, $D_c = 0.3$ m, 2 mm glass beads and polylobe extrudates three types of distributors (a) multi-orifice (b) bi-orifice (c)mono-orifice	(i) Maldistribution depends significantly on initial distribution (ii) Distribution is improved due to the presence of gas (iii) RTD is good method to determine the maldistribution as pressure drop can determine but cannot quantify it. Thermal sensors and tomography are too local and not realistic for every reactor
Li et al. (2000)	Liquid collector 64 cups	121 tubes 2 mm inside dia l = 100–300 mm d_p=1.6 mm trilobe particles	(i) Randomly packed bed with spherical and trilobe packings shows relatively uniform distribution (ii) Orientation effects in trilobe packing are canceled due to random packing (iii) The bed height improves the uniformity of the random packed bed (iv) Effect of gas velocity is not significant
Kundu et al. (2001)	Liquid collector six zones	$l = 0.152$ m Flow rate range $L = 1.46$–$7.31\,\mathrm{kg\,m^{-2}\,s^{-1}}$ $G = 0$–$0.043\,\mathrm{kg\,m^{-2}\,s^{-1}}$	(i) Decrease in surface tension and density reduces the wall flow (ii) Distribution improves with velocities (iii) Significant effect of particle geometry and orientation in case of cylindrical and other non-spherical shapes
Sederman and Gladden (2001)	Magnetic resonance imaging	$u_l = 0.5$–$5.8\,\mathrm{mm\,s^{-1}}$ $u_g = 66$–$356\,\mathrm{mm\,s^{-1}}$ $d_p = 5$ mm $D_c = 40$ mm	(i) Wetting efficiency increases with liquid flow rate (ii) No effect of gas flow rate on distribution (iii) Extreme liquid maldistribution in non-prewetted bed (iv) Start up procedure affects the final operating characteristics of TBR
Boyer and Fanget (2002)	Gamma-ray Tomography	$l = 60$ cm $d_p = 1.66$ mm $\varepsilon = 0.36$	(i) Flow is non axi-symmetric in several zones. This difference is attributed to bed structure (ii) Advocated the use of gamma ray tomography to study flow distribution in trickle-bed reactors