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A new model for bubbling fluidized bed reactors

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ABSTRACT

Various mathematical models have been proposed in the past for estimating the conversions of reactant gases in fluidized bed reactors. A new mathematical model is being proposed in this paper that gives relatively better results compared to the prevailing models for bubbling fluidized bed reactors utilizing Geldart B particles. The new model is named as JSR (Jain, Sathiyamoorthy, Rao) model and it is a modified version of bubble assemblage model of Kato and Wen (1969). This paper discusses the development of JSR model and its verification by using data from chemical engineering literature on fluidization and also experimental data from hydrochlorination of silicon in a fluidized bed reactor. The new model is tested for five processes having operating temperatures from 130 °C to 450 °C, operating velocities from 0.019 m s^{-1} to 0.19 m s^{-1} and solid particle sizes from 65 to 325 mesh.

Keywords: Fluidization; Modelling; Reactors; Powder; Particles; Compartments

1. Introduction

Initially two phase models consisting of bubble and emulsion phases and then three phase models having one more additional phase called cloud phase were proposed. Examples of two phase models are Davidson and Harrison (1963) and Patridge and Rowe (1966) models, and examples of three phase models are Kunii and Levenspiel model (1968) and Kato and Wen model (1969). Davidson and Harrison model had limitations with respect to high interphase mass transfer, and Patridge and Rowe model due to excess bubble-cloud area than actual. Therefore, both the two phase models could not provide satisfactory results. Models by Fryer and Potter (1972) and Werther (1980) were proposed. Fryer and Potter model is known as countercurrent back-mixing model (CCBM). The CCBM model did not become popular because of the difficulties associated with numerical solutions of the governing equations. The model used constant size bubble while it is a fact that bubble diameter changes as it rises in the fluidized bed. Werther (1980) model took an analogy from gas–liquid behaviour. In the this model the reactant gas from the gas phase to solid phase is assumed to be transported in a manner similar to the diffusion of a gas through a thin film into the bulk of a liquid in a gas–liquid interacting system. Kunii and Levenspiel (1968) and Kato and Wen (1969) models have been popularly used for design of bubbling fluidized bed reactors. There is still some scope for improvement for both these models as reported by Chavarie and Grace (1975). A new model (JSR, i.e., Jain, Sathiyamoorthy and Rao) has been proposed to improve and scale up the gas–solid bubbling fluidized bed reactors. The JSR model has been further tested using four reaction systems, viz. ammoxidation of propylene, hydrogenation of ethylene, oxidation of ammonia, decomposition of nitrous oxide by using data from chemical engineering literature. All the four reactions are confirmed to have first order as that of hydrochlorination of silicon metal. Experiments were carried out by us on hydrochlorination of silicon in a fluidized bed reactor in order to verify the predictions of the new JSR model. Silicon powder used in our experimental work belongs to classification Geldart B. The conversions of reactant gases in fluidized bed conditions are predicted utilizing JSR, Kunii and Levenspiel, and Kato and Wen models and compared.

1.1. Minimum fluidization velocity

Minimum fluidization velocity for classification Geldart B particles can be evaluated with a good accuracy from the correlation of (Delebarre, 2004)

$$24.5Re_{mf}^2 + 29,400\varepsilon_{mf}^3(1-\varepsilon_{mf})Re_{mf} = Ar \quad (1)$$

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Nomenclature

A	reactant gas
Ar	Archimedes number, $(d_p^3 \rho f(\rho_s - \rho_f) g/\mu_g{}^2)$, –
C_A	concentration of reactant gas in cloud phase, kg mol m^{-3}
C_e	concentration of reactant gas in emulsion phase, kg mol m^{-3}
C_b	concentration of reactant gas in bubble phase, kg mol m^{-3}
C_E	concentration of reactant gas at reactor exit, kg mol m^{-3}
C_o	concentration of reactant gas at entry of reactor, kg mol m^{-3}
C_{bh}	concentration of reactant gas in bubble phase at height h, kg mol m^{-3}
C_{bhi}	concentration of reactant gas in bubble phase at height h in ith compartment, kg mol m^{-3}
C_{En}	concentration of reactant gas at exit of nth compartment, kg mol m^{-3}
C_{En-1}	concentration of reactant gas at exit of $(n-1)$th compartment, kg mol m^{-3}
D	molecular diffusion coefficient of gas, m^2 s^{-1}
d_{bi}	initial bubble diameter, m
d_b	bubble diameter, m
d_p	particle diameter, m
d_t	reactor ID, m
d_{bm}	maximum bubble diameter, m
F	a parameter used in Eq. (5), –
g	gravitational acceleration, m s^{-2}
Δh_i	height of ith compartment, m
ID	internal diameter of reactor, m
K_{bc}	volume rate of gas exchange between bubble and cloud phases per unit bubble volume, s^{-1}
K_{be}	volume rate of gas exchange between bubble and emulsion phases per unit bubble volume, s^{-1}
K_{bei}	volume rate of gas exchange between bubble and emulsion phases in ith compartment per unit bubble volume, s^{-1}
K_{ce}	volume rate of gas exchange between cloud-wake and emulsion phase per unit bubble volume, s^{-1}
K_r	apparent fixed bed reaction rate constant, m^3/m^3 catalyst s^{-1}
K_f	apparent fluidized bed reaction rate constant, m^3/m^3 catalyst s^{-1}
L_{mf}	initial height of the solid bed, m
M	a parameter defined by Eq. (20)
t	time, s
Re_{mf}	Reynolds number at minimum fluidization velocity $(Re_{mf} = (d_p U_{mf} \rho f/\mu g))$, –
U_o,	superficial velocity of fluidizing gas, m s^{-1}
U_{mf}	superficial gas velocity at incipient fluidization, m s^{-1}
U_b	bubble velocity, m s^{-1}
U_{br}	bubble rise velocity, m s^{-1}
x	a parameter defined by Eq. (35) in appendix
X_A	conversion of reactant gas, –
X_{AJSR}	conversion of reactant gas by JSR model, –
X_{AKL}	conversion of reactant gas A by Kunii and Levenspiel model, –
X_{AKW}	conversion of reactant gas A by bubble assemblage model, –
α	a parameter defined by Eq. (9), –
β	a parameter defined by Eq. (12), –
γ_c	ratio of volume of solids in cloud-wake region to volume of bubbles in bed
γ_e	ratio of volume of solids in emulsion phase to volume of bubbles in bed
γ_b	ratio of volume of solids in bubble phase to volume of bubbles in bed
δ_I	bubble fraction of the HCl gas in the ith compartment
ψ	a parameter defined by Eq. (14), –
φ	a parameter defined in Eq. (22), –
ρ_s	density of solid particle, kg m^{-3}
ρ_f	density of the reactant gas, kg m^{-3}
ε_A	fractional change in volume between nil and complete conversion of reactant A
ε_{mf}	fraction of bed at incipient fluidization
μ_g	viscosity of the reactant gas, kg m^{-1} s^{-1}

or,

$$Re_{mf} = \left[\{600\varepsilon_{mf}^3(1-\varepsilon_{mf})\}^2 + 0.0408Ar\right]^{0.5} - 600\varepsilon_{mf}^3(1-\varepsilon_{mf}) \quad (2)$$

The above equation includes bed voids at minimum fluidization and helps better prediction of minimum fluidization velocity.

2. Development of an improved new mathematical model

Various phases in a bubbling bed model are shown in Fig. 1, and it is similar to Kunii and Levenspiel model. Three phases have been considered in the bubbling bed model. The model considers all bubbles of equal size throughout the bed and no counter-diffusion in the estimation of predicted conversion of the reactant. Kato and Wen (1969) have proposed a model in which a bubbling bed is divided into several hypothetical compartments of different sizes based on factors like particle density, gas velocity and particle diameter. New model brings important concepts of both Kunii and Levenspiel, and Kato and Wen models together.

Assumptions for new model

1. The model assumes bubbles of perfectly spherical shape.
2. It is assumed that in the cloud zone, wake is not a separate entity.
3. The reactant is assumed to diffuse from bubble phase to emulsion phase.
4. In any compartment the mass transfer is assumed to occur from a bubble of diameter equivalent to the compartment height. The emulsion phase is considered to be at incipient state of fluidization and considered to be well mixed up with constant voids.
5. The solid particles present in the bubble are neglected and hence the reaction with the gas in the bubble phase is assumed to be nil.

The model is discussed here in five steps as follows,

(i) Derivation of equation for compartment height