Chemical Engineering Science 176 (2018) 476–490

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

Modeling of complex liquid-solid flow of particle swelling in slurry loop reactors

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HIGHLIGHTS

- Particle swelling has significant influence on PE reactor operation.
- A heuristical model is developed to consider the aggregation of swelling particles in TFM.
- It captures the gradual increase of power consumption due to swelling in stirred tanks.
- It predicts slug formation and a sharp increase of power consumption in slurry loop reactors.
- It serves as a new way for reactor optimization.

ARTICLE INFO

Article history:
Received 18 June 2017
Received in revised form 3 November 2017
Accepted 8 November 2017
Available online 11 November 2017

Keywords:
CFD simulation
PBE
Polyethylene
Swelling
Loop reactor
Mesoscale

ABSTRACT

A swelling-dependent two-fluid model (STFM) is developed for the liquid-solid flows of swelling particles in polyethylene reactors. The model integrates the two-fluid model (TFM) with a species transport equation (STE) to account for the diffusion of alkane molecules from the liquid bulk to the amorphous region of particles, and a population balance equation (PBE) to consider the aggregation of swelling particles. Simulations show that only the TFM fails to capture the main features of swelling systems. By contrast, the STFM captures the gradual increase of power consumption due to particle swelling and aggregation, which agrees with the experiments in a stirred tank. The STFM predicts also the slug formation and a sharp increase of power consumption in a slurry loop reactor as well as the solid accumulation behind pump. The difference of model prediction for stirred tanks and loop reactors suggests the potential of reactor optimization by enhancing local mixing while still keeping high solid concentration for productivity.

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1. Introduction

Multiphase flow systems of swelling particles, e.g. water-clay systems, have been observed as complex systems with multiscale behavior, featuring the formation of the so-called mesoscale structures since 1990 s, as reported by Murad and Cushman (1996), Singh et al. (2003) and Cushman et al. (2004). Particle swelling complicates the multiphase flow rheology, which in turn has significant impacts on operation and performance of industrial reactors. Another typical example is the slurry loop reactors in ethylene copolymerization. In a typical slurry-phase polyethylene (PE) loop reactor, a liquid phase (diluent, monomer, co-monomer and hydrogen) and a polymer phase (polymer and sorbed quantities of diluent, monomer, co-monomer and hydrogen) coexist (Kufeld et al., 2006). The operating temperature has complex impacts on the chemical and physical behaviors in PE reactors, and is therefore an optimization variable. For example, it has to be set as high as possible to increase the catalyst productivity, but meanwhile high temperature also enhances the risk of swelling (Siraux, 2009). The preferable polymerization temperature in loop reactors is about 80 °C when producing the high molecular weight fraction (Touloupides, 2010). However, the local temperature cannot be perfectly controlled because of the reaction exotherm. Once the increasing temperature reaches a critical point, particle swelling occurs when the diluent, usually some kind of alkane, enters the polymer fluff and dissolves the low molecular weight polymers at microscale (often in molecular level), as illustrated in Fig. 1. The

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https://doi.org/10.1016/j.ces.2017.11.012
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Nomenclature

B_{agg}	birth rate due to aggregation, $m^{-4}\ s^{-1}$
D_{agg}	death rate due to aggregation, $m^{-4}\ s^{-1}$
G	growth rate, $m\ s^{-1}$
$\boldsymbol{J}_i$	the mass diffusion flux, $kg\ m^{-2}\ s^{-1}$
K_{ls}	liquid-solid drag coefficient, $kg\ m^{-3}\ s^{-1}$
L	particle diameter, m
m_{ls}	mass transfer from liquid to solid, $kg\ m^{-3}\ s$
m_2	2 th moment of number density function, m^{-1}
$n(L;\boldsymbol{x},t)$	number density, m^{-4}
N	agitation speed, rpm
P	pressure, Pa
P_s	pressure of solid phase, Pa
Po	power consumption, w
t_{ij}	the coalescence time, s
T	torque, J
$\boldsymbol{u_k}$	velocity vector of liquid or solid phase, m/s
Y_i	species i in the solid mixture phase, dimensionless

Greek letters

α_k	volume fraction of phase k, dimensionless
$\alpha_{s,avg}$	average solid volume fraction, dimensionless
ε	turbulence dissipation rate, $m^2\ s^{-3}$
ρ_k	density of phase k, $kg\ m^{-3}$
σ	surface tension, $N\ s^{-1}$
$\mu_{k,eff}$	effective viscosity of phase k, Pa s
λ_s	solids bulk viscosity, kg m/s
$\boldsymbol{\tau}_k$	stress of phase k, Pa
τ_{ij}	the contact time, s
ξ_{ij}	the ratio of the two particle diameters, dimensionless
Ω_{agg}	aggregation rate, $m^3\ s^{-1}$

Abbreviations

CFD	computational fluid dynamics
CSTR	continuous stirred-tank reactor
EMMS	energy-minimization multi-scale
KTGF	kinetic theory of granular flow
PBE	population balance equations
PE	polyethylene
STFM	swelling-dependent two-fluid model
STE	species transport equation
TFM	two-fluid model

Subscripts

l	liquid phase
s	solid phase in TFM or solid mixture phase in STFM

polymer slurry then tends to be more viscous or adhesive, generating a number of aggregates of polymer fluff at mesoscale. The particle aggregation may interfere the two-phase flow and eventually leads to reactor blockage or operational instability at macroscale (Fouarge et al., 2005; Siraux, 2009). Unplugging a fouled reactor is a time-intensive and costly undertaking (Benham et al., 1991). It is difficult, if not impossible, to ascertain the origin of particle swelling and quantify the aggregation behavior, and then evaluate the microscale and mesoscale impacts on multiphase fluid dynamics in PE loop reactors through pure experiments. Developing a swelling-based fluid dynamics model that is able to reasonably depict these effects is of practical significance for troubleshooting or optimizing such liquid-solid reactor systems.

There has been a large amount of experimental study on the fluid dynamics of liquid-solid flows in loop reactors or circulating fluidized beds. Liang et al. (1997) measured the solid holdup and

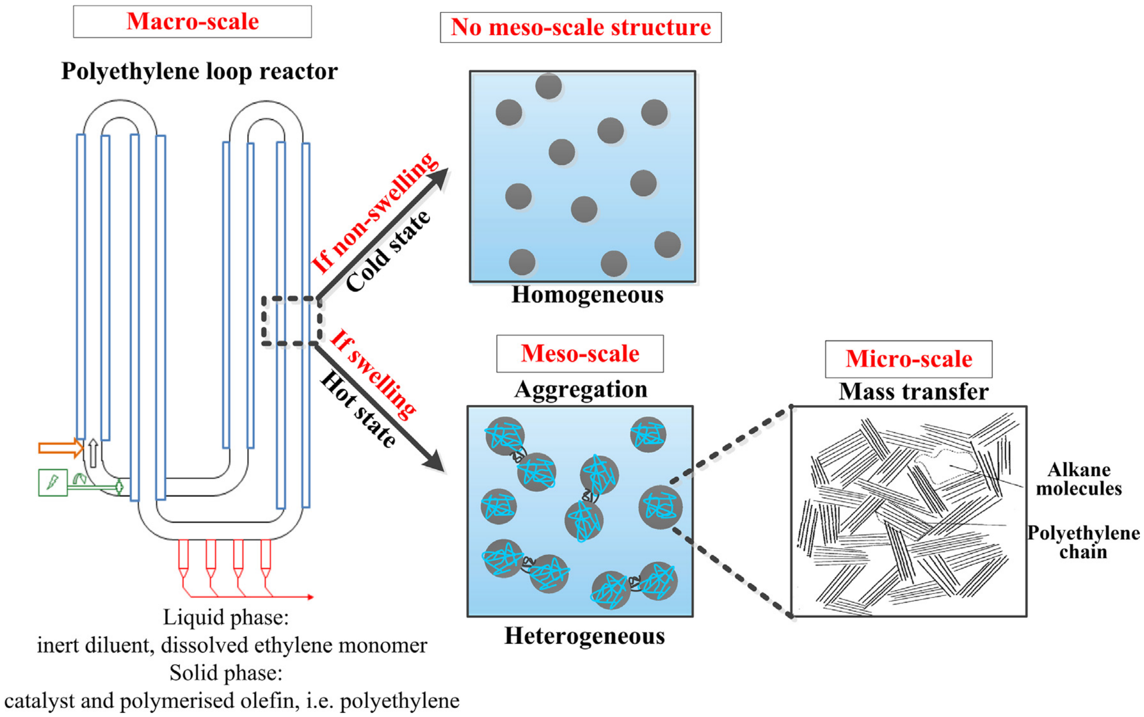

Fig. 1. Multiscale structures in a PE slurry loop reactor. (The blue fold lines in particles denote the absorbed alkane molecules and the black lines between particles denote the crosslinking of viscous polymers.) (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

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