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Population balance equations' application in rotating fluidized bed polymerization reactor

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ABSTRACT

Gas phase olefin polymerizations are now widely achieved in fluidized bed reactors. In fluidized bed poly-olefin reactors, small catalyst particles (20–80 μm) are introduced into the bed, and when exposed to the gas flow (monomer), polymerization occurs. At early stage of polymerization, the catalyst particles fragment into a large number of small particles then the polymer particles grow continuously, reaching a typical size of 1000–3000 μm. A successful analysis of this process not only should account for the kinetics of the polymerization but also should include the particles mixing and particle size distribution in the reactor.

Rotating fluidized bed reactors are the promising process to have a better control on the particle size distribution, particle separation and increasing the reactor efficiency. Due to the high rotational acceleration (e.g. 14 "*g*") that can be imposed in these kinds of reactors, our preliminary results showed that the amount of throughput, i.e. monomer flow rate, can be increased without worrying of changing the fluidization regime from well mixed condition to slugging, so the production rate and in consequence the polymerization yield will increase.

In this study the population balance approach is used to describe the evolution and growth of the particle size in gas–solid rotating fluidized bed olefin polymerization reactors along with CFD using Fluent program. The SMM (standard method of moments) method and QMOM (quadrature method of moments) method are used to solve the population balance equations; these are coupled with the conservation equations of mass and momentum for the gas and solid phases. Simulations have been performed with; a) constant particle growth rate and b) variable particle growth rate that is a function of polymerization reaction rate.

1. Introduction

Low-pressure gas phase polymerization is widely used for polymerization of ethylene and propylene in fluidized bed reactors. In spite of the significant application of this kind of reactors, they have shown limited flexibility in achieving high gas throughput because of the possibility of slugging and the inability to provide suitable heat transfer rates. To overcome these disadvantages and enhance the efficiency of the fluidized reactors, the feasibility of using the rotating fluidized bed reactors for this purpose is studied in this paper by using computational fluid dynamic (CFD) approach.

In brief summary, the gas-phase polymerization reaction in a fluidized bed begins when a catalyst particle, with a size of 15–100 μm in diameter is injected into the reactor. The gas phase monomer diffuses through the boundary layer around the catalyst particle and through its pores to reach the active sites, where the polymerization takes place. In few seconds, the pores of the catalyst support will fill up with the polymer. Then the support ruptures into many fragments, often called micrograins, microparticles or primary particles. Once the particles fragment, the volume of polymer inside the particle continues to grow as the monomer diffuses to the active sites. This process of expansion continues until the polymer particles exit the reactor; at which point they would have reached

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Nomenclature

A_t	total particle area (m^2)
$B(d_s; x, t)$	birth rate due to aggregation (m^{-4} s^{-1})
C_r	catalyst concentration
d_s	diameter of solid particle (m)
d_0	initial catalyst particle diameter (m)
d_{32}	Sauter mean diameter (m)
$D(d_s; x, t)$	death rate due to aggregation (m^{-4} s^{-1})
e_s	restitution coefficient
f	polynomial function
g	gravity acceleration (m/s^2)
g_0	radial distribution function
G	particle growth rate (m/s)
J_0	nucleation rate of particles (m^{-3} s^{-1})
k	moment order
k_a	area shape factor
k_v	volume shape factor
k_p	propagation rate constant
L_i	abscissas of the quadrature approximation (m)
m_k	kth moment of number density function (m^{k-3})
$\dot{m}$	mass transfer rate
M	monomer concentration
$n(d_s; x, t)$	length based number density function (m^{-4})
P	gas pressure (Pa)
P_s	solid pressure (Pa)
r_s	intrinsic polymerization rate (kg/(m^3 catalyst s))
Re_p	particles Reynolds number
S	mean stress tensor
t	time (s)
T_g	shear stress of gas phase
T_s	shear stress of solid phase
$\vec{u}_g$	Reynolds average velocity vector of gas phase (m/s)
$\vec{u}_n$	Reynolds average velocity vector of phase n (m/s)
$\vec{u}_s$	Reynolds average velocity vector of solid phase (m/s)
$\langle \vec{u}_{s\,i} \rangle$	particles Reynolds average velocity in the ith direction
$\vec{u}_s$	solid phase velocity vector
w_i	weight of the function f
x	coordinate direction

Greek letters

α_g	volume fraction of gas phase
α_n	volume fraction of phase n
α_s	volume fraction of solid phase
β	drag coefficient
Γ	molecular diffusivity
Γ_t	turbulent diffusivity
θ_s	granular temperature
λ_s	bulk viscosity of solid phase
μ_g	viscosity of gas phase
μ_s	viscosity of solid phase
ν	kinematics viscosity
ρ_g	gas density (kg/m^3)
ρ_n	density of phase n
ρ_s	particle density (kg/m^3)
Ω	angular velocity (rad/s)

Subscripts

g, s	gas, solid, respectively
n	phase

about 2000 μm in diameter. Since olefin polymerization is a highly exothermic, the heat generation rate can be very high inside the particles, which may lead to the appearance of hot spots. This occurs when the heat of polymerization cannot be efficiently removed through the porous polymer matrix and particle boundary layer to the bulk phase of the reactor. One of the major advantages of the fluidized bed reactor process is that the solid polymer particles are vigorously mixed in the reactor and by the fast flowing fluidizing gas, thus the heat of reaction can be removed more effectively (Choi and Ray, 1985a,b,c; Hutchinson, 1990; Tang et al., 1986; Chen, 1987).

In order to maintain reasonably high production rate, the gas-phase LLDPE (linear low density polyethylene) conventional fluidized bed reactor is operated at elevated temperatures, often approaching the softening temperature of the polymer product. Thus two main challenges must be resolved by any successful gas-phase polymerization process: (1) reducing the possibility of polymer particle sintering and agglomeration resulting from poor fluidization and poor heat removal, and (2) achieving good control of the polymer particle size distribution under a broad range of operating conditions. The control of particle size distribution is particularly important because it directly impacts the fluidizability of the polymer particles in the reactor (Chen, 1987).

In the conventional fluidized beds, fluidization occurs when the upward drag force balances the weight of the particles under gravity. Since the gravitational acceleration is a constant parameter, the minimum fluidization velocity is constant for particles with the same characteristic properties, i.e., particle diameter and density. Consequently, these systems are still limited to moderate throughputs because of the relatively low velocity required to fluidize the catalyst and polymer particles. On the other hand, rotating fluidized beds (RFBs) which has been recently investigated for similar processes provides added flexibility. These are evaluated in this article as an alternative technology, mostly because they permit higher flow rates. Since the particles in a RFB are fluidized in a controlled centrifugal field, the control of particles residence time would be improved as opposed to the constant gravitational force of the conventional fluidized bed.

In a rotating fluidized bed, the body force in a centrifugal bed becomes an adjustable parameter that is determined by the rotation speed and basket radius. By using a strong centrifugal field much greater than gravity, the particles in the bed will be able to withstand a high flow-rate without serious formation of large bubbles. The gas–solid contact is also expected to improve at a higher aeration rate. In a rotating fluidized bed of uniform particles (mono-size solid particles), unlike in a conventional fluidized bed, the granules are fluidized layer-by-layer from the gas–solid interface toward the side-wall distributor, as the inlet gas velocity is increased. This is a very significant and interesting phenomenon and is extremely important in the design of such fluidized beds (Chen, 1987; Ahmadzadeh et al., 2003; Arastoopour et al., 2004).

Qualitative and applied research was performed on rotating beds as early as the 1960s. Kroger et al. (1979, 1980) studied the effect of different parameters on the pressure drop in