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Effect of operating pressure on particle temperature distribution in a fluidized bed with heat production

Z. Li [a,b], M. van Sint Annaland [a,b], J.A.M. Kuipers [a,b], N.G. Deen [b,c,*]

[a] Multiphase Reactors Group, Department of Chemical Engineering & Chemistry, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands
[b] Dutch Polymer Institute (DPI), P.O. Box 902, 5600 AX Eindhoven, The Netherlands
[c] Multiphase & Reactive Flows Group, Department of Mechanical Engineering, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands

HIGHLIGHTS

- We present a systematic CFD-DEM study of fluidized beds at elevated pressure with heat production.
- These models can provide information on the particle temperature distribution.
- The effect of the pressure on *average* particle temperature can be attributed to the increased gas density.
- Changes in the bed hydrodynamics have an effect on the *spread* of the particle temperature distribution.

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ABSTRACT

The effect of elevated pressure on gas-solid heat-transfer behavior in an olefin polymerization fluidized bed was numerically analyzed by using an in-house developed 3-D computational fluid dynamics model coupled with a discrete element model (CFD-DEM). To mimic the heat generation associated with the polymerization reaction, a constant volumetric heat production was incorporated in the particle thermal energy equation. Snapshots of the heat transfer driving force (the difference between single particle temperature and average gas temperature) are presented to provide insight into the particle temperature distribution in the fluidized bed. Furthermore, it was found from the Probability Distribution Function (PDF) of the particle temperature that with increasing operating pressure the average particle temperature drops and the bed becomes more isothermal. Moreover, the average particle-gas heat transfer coefficient, was found to increase with increasing operating pressure. However, it is independent from the superficial gas velocity when the bed was operated above the minimum fluidization condition at the same elevated pressure. Predictive based on a continuous stirred tank reactor (CSTR) approximation of the bed reveals that the average particle temperature at steady state is determined by the inlet gas temperature, the temperature difference of the two phases and the adiabatic temperature rise. In polymerization reactors the adiabatic temperature rise is relatively high, therefore the effect of the pressure on the *average* temperature of the particles can be entirely attributed to the increased gas density, whereas changes in the bed hydrodynamics have an effect on the *spread* of the particle temperature distribution.

1. Introduction

Fluidized bed reactors (FBR) operated at elevated pressure are encountered in a variety of industrial processes such as fluidized bed combustion (Oka, 2003), coal gasification (McLendon et al., 2004), Fischer-Tropsch synthesis (Dry, 2002) and heterogeneous olefin polymerization, etc. From these processes the heterogeneous olefin polymerization benefits from operation at elevated pressure (up to 20 bar). Operation at elevated pressure offers several advantages such as improved bed-to-wall heat transfer (Jenkins et al., 1986), less particle segregation (Chen and Keairns, 1975a), and small reactor size (Chen and Keairns, 1975b). To optimize the highly exothermic olefin polymerization process conducted in FBR, fundamental knowledge of the hydrodynamics and heat transfer characteristics as a function of the operating pressure

* Corresponding author at: Multiphase & Reactive Flows Group, Department of Mechanical Engineering, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands.
E-mail address: N.G.Deen@tue.nl (N.G. Deen).

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Nomenclature

Symbols

a_s	Specific fluid-particle interfacial area, 1/m
A_B	Cross sectional area of the bed, m^2
C_d	Drag coefficient, dimensionless
C_p	Specific heat capacity of particle, J/kg/K
d_p	Particle diameter, m
d_{cell}	Length of grid cell, m
$\mathbf{g}$	Gravity, m/s^2
h	Effective interfacial heat transfer coefficient, W/m^2/K
k_g	Fluid thermal conductivity, W/m/K
k_g^{eff}	Effective thermal conductivity of the gas, W/m/K
$\mathbf{I}$	Unit tensor, dimensionless
m_a	Mass of individual particle, kg
N_p	Particle number in the bed, dimensionless
Nu_p	Particle Nusselt number, dimensionless
Pr	Prandtl number, dimensionless
p	Pressure, Pa
Q_p	Source term for the interphase heat exchange, W/m^3
$\mathbf{q}$	Heat flux, W/m^2
$\dot{q}$	Volumetric heat production, W/m^3
$\mathbf{r}_a$	Particle position, m
Re_p	Particle Reynolds number, dimensionless
$\mathbf{S}$	Body force exerted by particle on fluid, kg m/s^2
$\mathbf{T}_{contact,a}$	Particle torque, kg m/s
t	Simulation time, s
T	Temperature, K
$T_{p,m}$	Particle melting point, K
$\mathbf{u_g}$	Gas velocity, m/s
u_0	Superficial velocity, m/s
$\mathbf{v_a}$	Particle velocity, m/s
V_a	Particle volume, m^3
V_B	Volume of the bed, m^3
x	x direction, m
y	y direction, m
z	z direction, m

Greek symbols

ε	Volume fraction, dimensionless
ρ	Density, kg/m^3
τ	Newtonian stress tensor, N/m^2
μ	Dynamic gas viscosity, kg/(m s)
σ	Standard deviation of particle temperature, K
β	Inter-phase momentum coefficient, kg/m^{3}s
$\mathbf{\Theta}$	Particle angular velocity, rad/s

Subscripts

a	Individual particle
eff	Effective property
e	Emulsion phase
g	Property of gas
p	Property of particle
mf	Minimum fluidization
n	Time index
RD	Random packing

Superscript

∞	Properties at equilibrium state

is required. The influence of pressure on the bed hydrodynamics has been investigated by utilizing several experimental methods, i.e. with the use of electrical capacitance tomography (ECT) and X-ray tomography (Sidorenko and Rhodes, 2004; Yates and Simons, 1994). On basis of experimental studies it has been reported that the hydrodynamic characteristics of fluidized beds strongly depend on the operating pressure (Chan et al., 1987; Chitester et al., 1984; Olowson and Almstedt, 1990), i.e. the minimum fluidization velocity (Olowson and Almstedt, 1991), bubble characteristics such as growth, size and pathway in the bed (Sidorenko and Rhodes, 2004; Yates, 1996), etc.

In the past decades, due to the ongoing development of computational technology, the effects of pressure on the hydrodynamics of FBR have been investigated in detailed using CFD approaches. Li and Kuipers (2002) investigated the pressure effect with a CFD-DEM model, where they found that an elevated pressure reduces the incipient fluidization velocity, while the window (i.e. gas velocity range) for uniform fluidization increases. It narrows down the bubbling regime and leads to a quick transition to the turbulent regime. They also observed that an elevated operating pressure suppresses bubble growth and therefore produces more uniform gas-solid flow structures. A number of key features for fluidized beds, such as the bubble behavior, flow patterns, solids mixing and particle granular temperature have been investigated by Godlieb et al. (2008) using state-of-art CFD-DEM simulations. They reported that at elevated pressure, the gas-particle interaction is enhanced and becomes relatively more important as compared to the particle-particle interaction. The bubble size also decreases, whereas bubble breakage becomes more pronounced. Solids mixing is also enhanced at elevated pressure condition. It is noticed that most of these studies describe the effect of elevated pressure on the hydrodynamics of fluidized bed, while very little research has been published on the changed gas-particle heat transfer behavior or the combination of these two aspects. It is known that elevated pressures can enhance the wall-to-bed heat transfer (Borodulya et al., 1991; Yew Looi et al., 2002) in fluidized beds, however, there is a lack of detailed information of the pressure effect on gas-particle heat transport. The increase of the heat transfer rate at elevated pressure can directly be related to the increased density of the gas. So, one can directly use the gas properties at elevated pressure to simulate the heat transport in a fluidized bed, like was done in the work of Kaneko et al. (1999). The gas properties (in particular the gas density) at elevated pressure conditions were used to mimic the conditions of elevated pressure to calculate the heat transfer coefficient. However, the effect of the pressure on the hydrodynamics was not considered in these simulations. Therefore, in this paper we will study the effect of pressure on the heat transport in fluidized beds considering both the effect of the increased density and the effect of the altered hydrodynamics.

This work is organized as follows. First details of the governing equations of the CFD-DEM are given. A constant heat source for mimicking the heat generation due to the strongly exothermic polypropylene polymerization has been incorporated in the particle thermal energy equation using an estimated value from literature (Choi and Ray, 1985). In the results and discussion section, the hydrodynamics is characterized in terms of snapshots of bubble behavior, time-averaged solids circulation patterns and the time-averaged probability distribution function (PDF) of the bed porosity. Subsequently, the particle temperature PDF of mono-