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Numerical simulation and experimental verification of gas flow through packed beds

S. Natarajan[a], C. Zhang[a,*], C. Briens[b]

[a]Department of Mechanical and Materials Engineering, The University of Western Ontario, London, Canada N6A 5B9
[b]Department of Chemical and Biochemical Engineering, The University of Western Ontario, London, Canada N6A 5B9

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Abstract

This study is concerned with an industrial application involved in the manufacture of the polymer Nylon12 which is polymerised from solid monomer particles. There exists interstitial air among those particles. Oxygen in the air is a strong inhibitor of the polymerization reaction and has to be eliminated from the packed bed of monomer particles before they are introduced into the polymerization reactor. This is done by injecting nitrogen into the packed bed from the bottom of the bed. The nitrogen spreads into the packed bed and displaces the interstitial air. This process is already being employed in the polymer processing industry. The present research focuses on how to make this oxygen elimination process more effective.

Using a numerical method to optimize parameters that affect the oxygen elimination process in packed beds, such as the number of injection jets, their positions and angles, etc., saves time and reduces cost. However, the numerical model needs to be validated before carrying out such a parametric study. Therefore, the experiments on the fluid flow in a packed bed are conducted to validate the numerical model. The numerical model is also validated against the analytical results for a packed bed with simplified geometry. The numerical results agree well with the experimental data and the analytical results. The gas flow through packed beds is treated as flow through a porous medium. The resistance to the flow due to the presence of the porous medium is represented by an additional momentum sink in the Navier–Stokes equations.

Keywords: Diffusion; Laminar flow; Packed bed; Porosity; Porous media; CFD

1. Introduction

Fluid flow and heat transfer analysis through packed beds is a common occurrence in the field of chemical engineering. Mostly, the studies on packed beds so far have focussed on the porosity distribution and heat transfer phenomena. The literature for these two areas is extensive and a few examples are discussed here. The work of Benenati and Brosilow [1] was one of the first to analyze voidage distribution in randomly packed beds. Wang et al. [2] studied the porosity distribution using the gamma ray tomography technique. Dixon and van Dongeren [3] studied the influence of the tube and particle diameters at constant ratio on heat transfer in packed beds.

Dixon and Nijemeisland [4] reviewed the use of computational fluid dynamics (CFD) as a design tool for fixed bed reactors. FLUENT™ was used for their simulations. They reviewed the classical and more recent approaches used in the modeling of packed beds. Yin et al. [5] conducted CFD modeling of mass-transfer processes in randomly packed distillation columns. Their model took into consideration the radial and axial variations in flow and mass transfer. Their results were in good agreement with the experimental results. They used volume-averaged fluid dynamics equations and closure models to account for drag forces, body forces, interface mass transfer, etc. These closure models were pre-existing empirical correlations like Leva's correlation, Robin's correlation, etc. They solved the governing equations numerically using the CFD package CFX™.

Logtenburg and Dixon [6] and Logtenburg et al. [7] mainly dealt with heat transfer analysis in packed beds using CFD techniques. Zeiser et al. [8] used Lattice-Boltzmann

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* Corresponding author. Tel.: +1 519 661 2111x88345; fax: +1 519 661 3020.

E-mail address: zhangc@engga.uwo.ca (C. Zhang).

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method to analyse the flow field and pressure drop in packed beds. Their work also focussed on packed beds of low aspect ratio. Ewing et al. [9] presented a numerical method for the modeling of multi-component gas flow in porous media. They used the Forchheimer's equation to model non-Darcy flow, which is believed to be more accurate than the classical Darcy's equation for high-speed gas flow. Forchheimer's equation was discretized using a finite-element method.

The present work seeks an effective way to eliminate oxygen from a packed bed of monomer particles. This process finds application in the polymer processing industries involved in the manufacture of Nylon12. In the manufacture of the polymer Nylon12, the polymerization reaction is hindered by the presence of oxygen. The ultimate purpose of this study is to improve oxygen removal from a packed bed through parametric studies. Numerical simulation is an efficient way to conduct parametric studies due to its low cost and rapidity.

The numerical approach used to model the fluid flow in the packed bed, however, needs to be validated against the experimental data. The conventional approaches for a parametric study of a packed bed, such as conducting experiments on an experimental packed bed and using the axial dispersion model (ADM), have their own disadvantages. Scale-up criteria for experimental results are unknown, while the ADM cannot be used for packed beds with complex geometries. Since the effect of the variations of the velocity and pressure of the gas phase in the packed bed on the gas-phase concentration change is not included in the ADM, it can be used only for packed beds with simple geometries. Also, the ADM can handle only perfect gas distribution, i.e., uniform gas flow at the bottom of the packed bed, which is not possible in most practical packed beds, the reason being the solid monomer particles have to flow unimpeded from the bottom of the packed bed into the polymerization reactor. Therefore, the gas has to be injected into the packed bed through individual injection nozzles located on the side of the packed bed. The numerical approach presented in this work uses the fundamental laws for fluid flow. Therefore, there is no scale-up problem and it can be used for packed beds with complex geometries.

Nitrogen, which is used to purge out the oxygen, does not interact with the monomer particles and hence there is no chemical reaction or adsorption involved in this process. The process takes place at atmospheric temperature and pressure. The fluid flow inside the packed bed is a multi-component gas flow through a porous medium. The numerical simulations are carried out using FLUENT™ [10].

2. Configuration of the experimental packed bed

Fig. 1 shows the configuration of the experimental packed bed used in this study. The cylindrical section of the packed bed is 0.280 m in diameter and 0.540 m in height. The cone has an included angle of 18° and a bottom diameter of 0.05 m. Four injectors used for nitrogen injection are of 3.175×10^{-3} m in diameter and are connected to the cone region of the packed bed from a vertical distance of 0.19 m from the bottom of the cylindrical section. The jets are at right angles to each other positioned downward and parallel to the cone wall. The bed is filled with monomer particles. The voids in between the monomer particles in the packed bed initially contain air. Nitrogen is injected into the packed bed through the four injectors to eliminate the air.

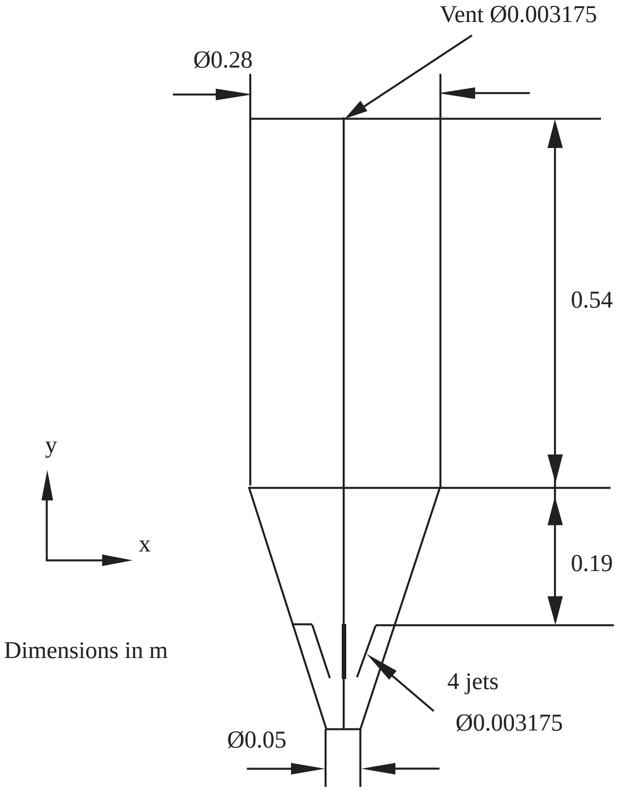

Fig. 1. Configuration of the packed bed.

The flow rate, and hence the velocity of the carrier gas, which is the gas injected into the packed bed, is restricted by the requirement that the superficial velocity in the packed bed should be much lower than the minimum fluidization velocity of the monomer particles. The fluidization velocity is the velocity beyond which the solid monomer particles start moving. When the particles are fluidized, they can move over the whole bed volume, which leads to undesirable back mixing of both gas and solid phases.

The superficial velocity (Us) is defined as the ratio of the volumetric flow rate of the carrier gas to the cross-sectional area of the packed bed, i.e.

$$U_s = Q/A_c \tag{1}$$

The minimum fluidization velocity (U_{mf}) of monomer particles in the packed bed is given by Leva's correlation [11],

$$U_{mf} = 7.169 \times 10^{-4} g D_p^{1.82} (\rho_p - \rho_g)^{0.94} / \rho_g^{0.06} \mu_g^{0.88} \tag{2}$$

The density and the Sauter-mean particle diameter of non-porous monomer particles in the packed bed are 1040