Numerical Simulation for the Wall Channeling of Packed Bed in the Chemical Industry

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Abstract. Wall channeling has a significant impact on the profiles of flow velocity in packed bed. Using fore treatment software GAMBIT, the three-dimensional packed bed model was established. Grids of three-dimensional model were divided by the means of coin division. Based on FLUENT porous media model, the anisotropy of radial porosity in packed bed was reflected with the User Defined Functions of FLUENT. The profiles of flow velocity in packed bed with anisotropy and isotropy of radial porosity were compared. In the condition of anisotropy, the effects of the particle diameters on wall channeling were analyzed by comparing the flow and distribution regular pattern inside the packed bed with different particle diameters. The analytic results showed that the velocity near the wall was larger than the center region for the anisotropy of radial porosity. Under the same conditions, the width of affected area could be decreased if smaller particles were used, but the maximum of velocity in affected area was bigger than larger particles.

Introduction

The porosity of the packed bed in the chemical industry is an important feature of the packed bed. Due to the impact of the bed wall near the wall, the porosity of the bed may change sharply, and is very different from the porosity distribution away from the wall, which directly affects the flow distribution of the fluid[1]. In fact, the bed porosity near wall surface is greater than that of the internal of the bed, more fluid tends to flow through near the wall, which makes the upper bed-sectional velocity distribution be uneven and this phenomenon is known as wall effects[2]. Wall effect has an important effect on mass and heat transfer of packed bed[3]. For example, for pressure swing adsorption packed bed, wall effects may lead to a mixed gas early penetrate from near the wall in the adsorption process, to reduce the concentration of gas exports, and for the fixed packed bed reactor, the wall effect will affect the conversion rate of reaction and yield and quality of products[4-6]. In the past three decades, a large number of experimental studies on the packed bed have been made, and based on this an empirical model has been established, which are one-dimensional model[7]. For the traditional one-dimensional plug flow model that considers only the axial transfer flow, regardless of the radial distribution difference between bed porosity, ignoring the opposite sex of radial flow velocity, temperature and concentration of the fluid in the packed bed[7,8]. However, in guiding the packed bed design, especially when it is a large diameter and low radial bed and radial flow packed bed, it must consider the porosity distribution of packed bed. Consider the radial anisotropy of bed porosity, it is very important for the evaluation of the performance of the packed bed [9-11].

The applicable range of porous media model in FLUENT software of Computational Fluid Dynamics (CFD) is very wide, such as the simulation analysis of packed bed, perforated plate, flow distribution, etc[12]. Currently, specialized computational fluid dynamics method study in wall effect is reported little, and empirical models established based on experiments think that the beds are isotropy, one-dimensional flow model of the piston. As to the shortage of one-dimensional piston flow model, use porous media model in FLUENT to establish three-dimensional packed bed model, through a user-defined function (UDF), the performance of the radial distribution inhomogeneity of bed porosity, we research the radial distribution anisotropy influence of porosity on the bed flow field, also the influence of filler particles diameter on the wall effect is discussed.

Geometric model and mathematic model

The two-dimensional cross-sectional geometry of vertical packed-bed is shown in Figure 1, the import and export diameters of gas are Φ50mm, the bed diameter is Φ100mm, bed of porous zone is 400mm high, fluid uses air with constant density, packed bed particles are spherical.

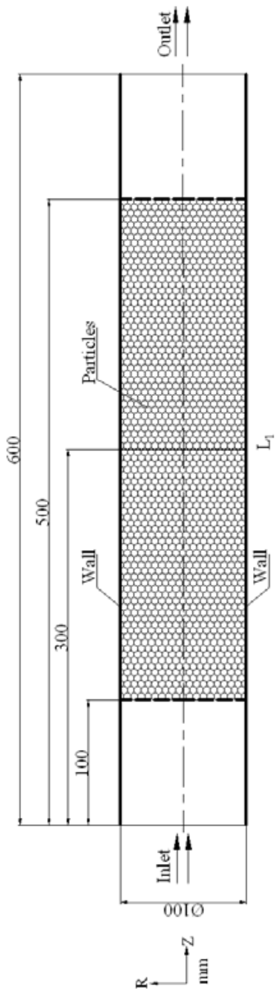

Fig. 1 Two-dimension geometry model of packed bed

Basic equation

Porosity and drag coefficient of porous media model is introduced on the basis of the basic equations of fluid mechanics, which is used to describe fluid flow in porous media regions. Whereby the mathematical model of packed bed fluid flow is obtained, the basic equation of which is consisted of mass conservation equation and momentum conservation equation.

Mass conservation equation:

$$\nabla(\varepsilon\rho_f \vec{v}) = 0 \qquad (1)$$

Where, ρ_f , ε , $\vec{v}$ respectively are gas density, the porosity of the bed and the velocity vector.

Momentum conservation equation:

$$\nabla(\rho_f \varepsilon \vec{v}\vec{v}) = -\varepsilon\nabla p + \nabla(\varepsilon \overline{\overline{\tau}}) + \vec{F} \qquad (2)$$

Where, p static pressure, $\overline{\overline{\tau}}$ is stress tensor, $\vec{F}$ is additional resistance term generated by porous medium.

Additional resistance term generated by porous medium

When fluid flows through a packed bed of solid particles, it will face inertial resistance and viscous resistance which generated attenuation. In porous media model of FLUENT software, by adding momentum source to the momentum conservation equation to express momentum attenuation, additional resistance term $\vec{F}$ can be calculated as follow:

$$\vec{F} = -\mu \frac{\vec{v}}{\alpha} - C_2 \rho_f \left|\vec{v}\right| \vec{v} \qquad (3)$$

$\frac{1}{\alpha}$ represents the viscous drag coefficient, C_2 represents inertial resistance coefficient. α and C_2 is calculated by Eugen equation of fixed bed [13]:

$$\alpha = \frac{d_p^2 \varepsilon^3}{150(1-\varepsilon)^2}, \quad C_2 = \frac{1.75(1-\varepsilon)}{d_p \varepsilon^3} \qquad (4)$$

Bed porosity distribution and treatment

(1) Adopt the equation Nield and Beian gave to calculate radial porosity distribution of the packed bed [14].

$$\varepsilon = 0.4[1+1.4\exp(-5y/d_p)] \qquad (5)$$

Where, y denotes the distance from the ground, d_p represents the particle diameter.

(2) Processing Method

Use C_CENTROID(x,c,t) in FLUENT to get centroid coordinate of grid cells, DEFINE_PROFILE((c,t,i) is used to define the bed porosity, porous medium drag coefficient (including the viscous drag coefficient and the inertial resistance coefficient). At the same time, use user-defined scalar (UDS) to define the bed porosity for porosity information storage of each unit at the centroid in porous zone, as an intermediate variable to the formula (4) in computing the porous zone at each point of the drag coefficient after treatment, the porosity of custom programming add panel is shown in Figure 2.

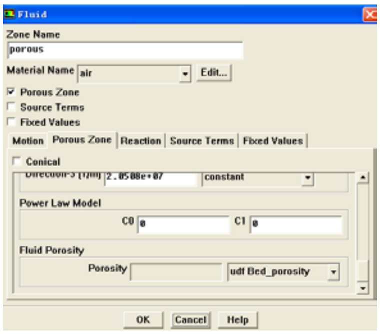

Fig. 2 The control panel for the addition of porosity

Model parameters and boundary conditions

Fluid, solid particle and boundary conditions are shown in Table 1.

Table 1 Model parameters and boundary conditions

Parameter	Value	Parameter	Value
ρf (kg·m-3)	1.16	*P*(pa)	101325
μ(Pa·s)	1.84×10^{-5}	d_p(mm)	5～20
Velocity inport (m·s-1)	0.1	Pressure export(Pa)	101325
Bed wall	No-slip insulation wall	Packed beds	Axisymmetric

Meshing and calculation method

Use special pre-processing software GAMBIT to establish three-dimensional axisymmetric packed bed geometry, and use coin division method to generate hexahedral grid cells, and the grid near the wall is encrypted, as is shown in Fig. 2, and the hexahedral grid cell number is 24604712.

Based on the discrete control equation of finite volume method, pressure and velocity equation coupled use SIMPLE algorithm, double steady implicit solver is used to solve using PRESTO discrete pressure, second-order upwind discrete momentum, and the convergence criterion is that the residual value of each differential equation is less than 10^{-5}.

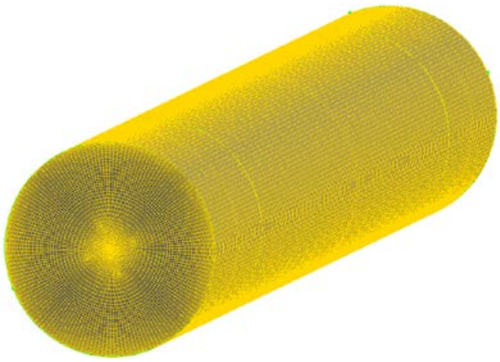

Fig.3 Grids of three-dimensional model

Results and analysis

Based on the above-mentioned geometric and mathematical model, when the particle diameter is 5mm, the comparative analysis and simulation of packed bed whose radial anisotropy and porosity isotropy porosity is constant 0.4 are done. By changing the diameter of the filler particles, the influence of filler particle diameter on wall effect is explored.

Radial distribution of porosity

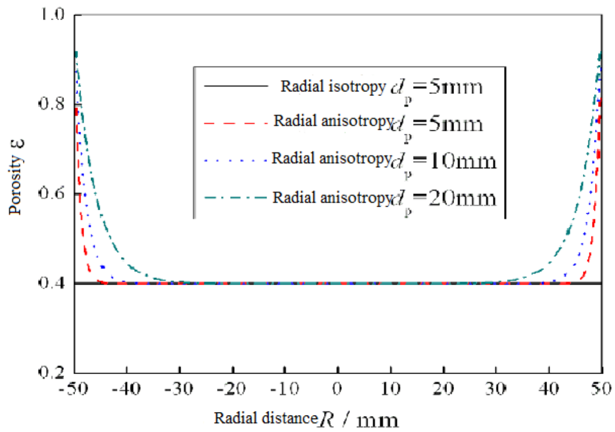

Fig.4 the radially varying of porosity along L_1

Figure 4 shows the radially varying of porosity along L_1 when considering radial anisotropy of porosity and different particle diameters. As can be seen from the figure, at the same bed diameter, when the particle diameter is 5mm, near the wall, the bed porosity taking radial anisotropy into account is 0.8 or more, which is very different from the 0.4 porosity value of radial isotropy. Under the same bed diameter, the smaller the particle diameter is, the narrower the bed porosity change region near the wall is, and the less obvious porosity radially anisotropy is.

Porosity distribution influence on the velocity distribution of cross section. Figure 5 shows contour plots of the velocity profile for the section of Z=300mm in different distribution of porosity. As can be seen from the figure, at the same import gas flow rate, when the particle diameter is 5mm, near the wall, the maximum of flow rate to considering porosity radial isotropy can be up to 0.494m/s, bed-sectional velocity distribution of radial porosity isotropy is uniform, at about 0.250m/s or so, vary greatly. When particle diameter is 5mm, 10mm and 20mm, the maximum of velocity near the wall are 0.494m/s, 0.425m/s, 0.352m/s. In Fig. 5, the area of flow rate changing dramatically is subject to the effect of the wall area. Compare the speed cloud of different particle diameters, and it can be found under the same outer diameter and inlet gas flow rate, the smaller the particle diameter is, the larger the maximum value of flow rate near the wall, but the narrower the wall effect influence area is.

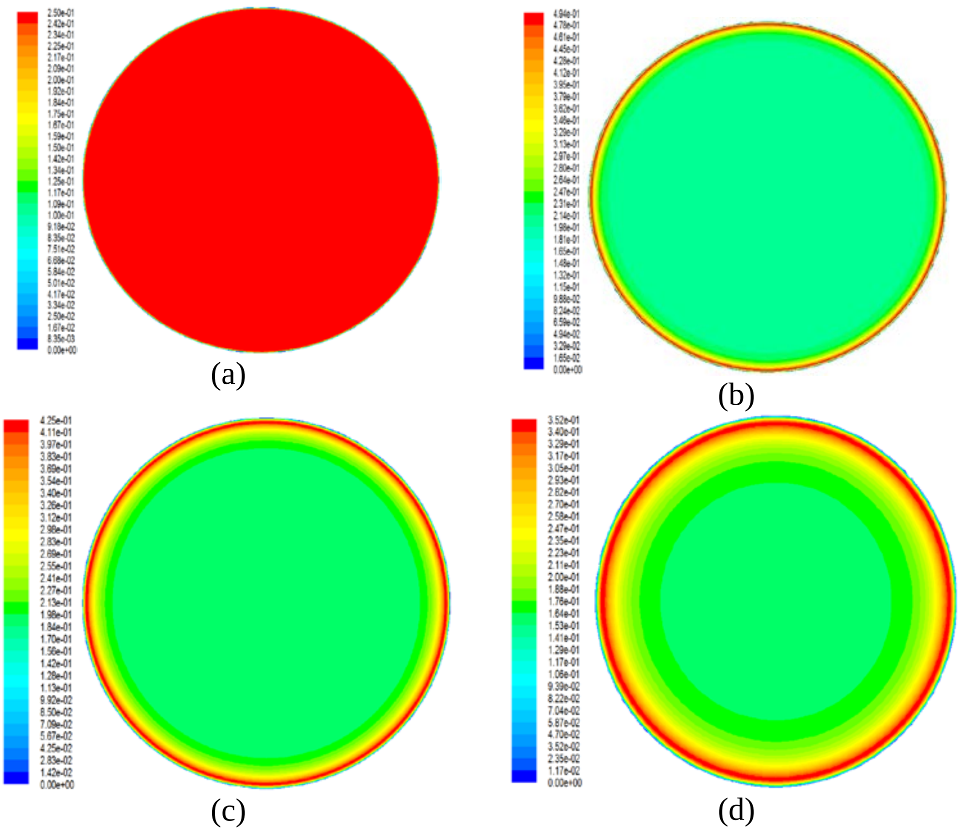

Fig.5 Contour plots of the velocity profile for the section of Z=300mm in different distribution of porosity, (a) Isotropy with dp=5mm, (b) Anisotropy with dp=5mm, (c) Anisotropy with dp=10mm, (d) Anisotropy with dp=20mm,

Porosity distribution influence on the flow velocity. To further illustrate the porosity radial anisotropy influence on the velocity of the bed wall and wall effects under different particle diameter, compare L_1 and it can be obtained that the flow rate is as shown in Fig. 6. As it can be seen from the figure, for the bed considering porosity radial anisotropy, the velocity near the wall is larger than that in the middle of the bed. Since the wall friction velocity drops to zero at completely close the wall, which is due to the bed porosity near the wall is greater than that of the middle of the bed, more fluid tends to flow through near the wall. Considering the bed porosity radially anisotropy, compare the flow velocity profiles under different particle diameters, it can be found that the larger the particle diameter is, the smaller the flow rate of the bed in the middle region is, the smaller the maximum value of flow rate near the wall is, but the wider the wall effect area is. This is due to that under the same inlet velocity condition, the wall effect area using the bed of large diameter particles is wider, more fluid flow from the area the wall effect acts, so the flow rate in the middle of the bed is smaller. For the bed using small particle, the resistance coefficient is greater, more fluid tends to flow over from near the wall, and therefore there is a maximum velocity near the wall, because the effect area of the wall effect is so narrow that the flow rate of small particles bed in the middle region is larger than that of large particles bed.

Conclusion

The radial inhomogeneity of bed porosity has an important influence on the distribution of fluid, and the radial anisotropy of bed porosity will cause the flow rate of the bed near the wall increase sharply, which is greater than the phenomenon of the central region of the bed so that the bed cross-sectional flow rate is unevenly distributed. Under the same conditions, the bed using small particles can reduce the area width of wall effect, but the drag coefficient of the bed will increase, which leads that the flow rate maximum of bed near the wall is bigger than that of the large particles bed, and fluid is easier to penetrate bed.

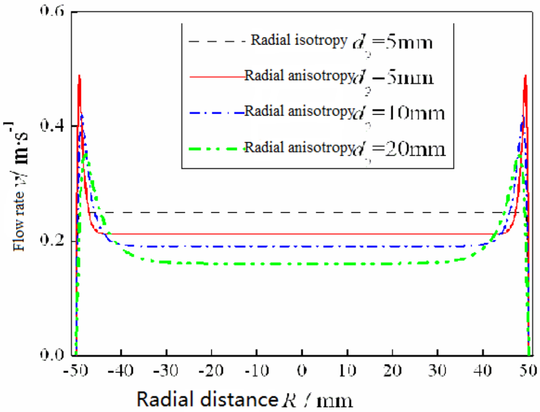

Fig.6 The velocity radial profile along the L1 in different distribution of porosity

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