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COMPARISON OF SEVERAL TURBULENCE MODELS APPLIED TO THE SIMULATION OF GAS FLOW IN A PACKED BED

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ABSTRACT

In this paper, three turbulence models for porous media are applied to the gas flow through a randomly packed bed and are validated by means of a parametric study and by comparison with experimental data in literature. These models predict widely different turbulent eddy viscosity, with the model by Nakayama & Kuwahara (1999) being the best in predicting a reasonable eddy viscosity. Residence time distribution (RTD) and velocity distribution are then simulated by considering a radial profile of porosity, and the results are in good agreement with the available experimental data.

NOMENCLATURE

$a_{1\text{-}4}$ constants for porosity expression,-
C scalar concentration, kmol/m^3
c_μ, c_1, c_2, c_k turbulence model constants,-
d_p particle diameter, m
D molecular diffusivity coefficient of tracer, m^2/s
D_{ax} axial dispersion coefficient in plug flow model, m^2/s
K permeability, m^2/s
k turbulent kinetic energy, m^2/s^2
k_∞ turbulence model constant, m^2/s^2
l bed length, m
Pe Peclet number defined by Eq.(13), -
R_0 resistance coefficient, Ns/m^4
Re_p particle Reynolds number, $Re_p = \dfrac{\rho U d_p}{\mu}$
S_k source terms in k equation, N/(m^{2}s)
S_ε source terms in ε equation, N/(m^{2}s^2)
Sc Schmidt number, $\mathrm{Sc} = \dfrac{\mu}{\rho D}$
t real time from tracer injection, s
U artificial velocity, m/s
u interstitial velocity, m/s
$\mathbf{u}$ interstitial velocity vector, m/s
y distance to the wall normalised by d_p, -
Z axial position normalised by l,
θ dimensionless time with respect τ,-
ε turbulent dissipation rate, m^2/s^3
ε_∞ turbulence model constant, m^2/s^3
σ turbulent Prandtl number (=0.9)
μ laminar viscosity, Ns/m^2
μ_t turbulent eddy viscosity, Ns/m^2
γ volume porosity, -
τ mean residence time, s

INTRODUCTION

Many processes in the chemical and metallurgical industries involve flow of fluids in packed beds. Mathematical modelling of such flow and related phenomena is useful in enhancing the performance of these processes. To date, most of the models proposed are based on the assumption of plug flow and do not take into account maldistribution. However, it is well known that in unstructured fixed beds, the void fraction in the vicinity of the containing wall approaches unity and displays a decaying oscillation profile with the distance from the wall (Mueller, 1992). Daszkowski and Eigenberger (1992) have shown that reaction and radial heat transfer can be modelled correctly, only if radial inhomogeneities are properly considered.

The radial distribution of velocity follows the permeability profile due to the variation of the resistance force. An oscillatory velocity profile, although not easily visible from the RTD of a tracer (Paterson et al., 2000), has been observed both at immediately downstream of the packing bed (Bey and Eigenberger, 1997; Subagyo et al., 1998) and inside the bed (McGreavy et al., 1986; Stephenson and Stewart, 1986).

Direct simulation of the detailed microscopic flow of the clear fluid within the voids between packed particles is still impractical, but the volume-averaged flow field can be described by the Navier-Stokes equations if additional terms for fluid-particle interactions are incorporated. Vortmeyer and Schuster (1983) proposed the application of the extended Brinkman equation where the fluid-particle interaction was described by a two-dimensional Ergun pressure drop correlation and wall friction was separately taken into account. Momentum equations for interstitial velocity were normally used assuming laminar viscosity (Delmas and Froment, 1988). Bey and Eigenberger (1997) showed that a turbulent viscosity is more appropriate. By employing an effective viscosity as an adjusting factor, Ziolkowska and Ziolkowski (1993) and Bey and Eigenberger (1997) tried to develop a mathematical model of velocity distribution.

In the mathematical or numerical models mentioned above, there are a number of assumptions or tuning parameters to fit to the measured data under a particular set of operating conditions, thus lacking generality for general engineering applications. A turbulence model is useful in determining the unknown parameters that appear in the basic transport equations. The recent progress of turbulence models in porous media makes it possible to numerically model a wide range of applications directly. A review of such models can be found in de Lemos and Pedras (2001). In most of these models, macroscopic model equations are derived from the microscopic flow equations by a form of volume averaging, and extra source terms arise in the model equations due to the solid particles. These source terms were commonly formulated based on numerical experiment results from certain two-dimensional (particularly periodic fully developed, unidirectional) porous matrixes, such as periodic arrays of rods. These models have rarely been validated in three-dimensional porous structures, i. e., validation against a range of three-dimensional porous media, like randomly packed spheres, is required.

This paper compares three recently published turbulence models (Takeda, 1994; Nakayama and Kuwahara, 1999; Pedras and de Lemos, 2001) applied to a simple isothermal packed column of spheres. It will be shown that a CFD model facilitated with a proper turbulence model is capable of simulating the flow in such packed beds.

MODEL EQUATIONS

The steady state form of mean flow equations in an isotropic porous medium can be written as,

$$\nabla\cdot(\rho\gamma\mathbf{u})=0 \tag{1}$$

$$\nabla\cdot(\rho\gamma\mathbf{u}\mathbf{u})-\nabla\cdot(\mu_{eff}(\nabla(\gamma\mathbf{u})+(\nabla\gamma\mathbf{u})^{\mathrm{T}})) = -\gamma\nabla p-\gamma R_0\mathbf{u} \tag{2}$$

$$\mu_{eff}=\mu+\mu_t \tag{3}$$

$$\mu_t=\rho c_\mu\frac{k^2}{\varepsilon} \tag{4}$$

which is similar to the Reynolds averaged Navier Stokes equations with an eddy viscosity accounting for the turbulent effect. The last term in Eq.(2) represents a resistance to flow in the porous medium. Based on Ergun's equation, the resistance coefficient for a flow through a bed of smooth spheres is given by,

$$R_0=150\mu\frac{(1-\gamma)^2}{\gamma^2 d_p^2}+1.75\rho\frac{1-\gamma}{\gamma d_p}|\mathbf{u}| \tag{5}$$

The turbulence model equations based on the standard k-ε model run as,

$$\nabla\cdot(\rho\gamma\mathbf{u}k)-\nabla\cdot\left[(\mu+\frac{\mu_t}{\sigma_k})\nabla(\gamma k)\right] = \gamma\mu_{eff}\nabla\mathbf{u}\cdot(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)+\gamma S_k-\rho\gamma\varepsilon \tag{6}$$

$$\nabla\cdot(\rho\gamma\mathbf{u}\varepsilon)-\nabla\cdot\left[(\mu+\frac{\mu_t}{\sigma_\varepsilon})\nabla(\gamma\varepsilon)\right] = c_1\gamma\mu_{eff}\nabla\mathbf{u}\cdot(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)\frac{\varepsilon}{k}+c_2\gamma\left[S_\varepsilon-\rho\frac{\varepsilon^2}{k}\right] \tag{7}$$

These macroscopic turbulence model equations, in contrast with the microscopic k-ε equations, present two extra terms, i.e., S_k and S_ε that represent extra transport/production of turbulence kinetic energy and its dissipation due to the presence of the porous media. The source terms vary in formulation (Takeda, 1994; Nakayama and Kuwahara, 1999; Pedras and de Lemos, 2001) and are listed in Table 1. The values of these sources vanish for the limiting case of no packing material present, or say, when the porosity $\gamma\to 1$, meaning that the normal k-ε model equation is recovered.

We choose these three models because of their relative simplicity and completed closure. Validation of other models is the subject of future work.

	S_k	S_ε
Nakayama & Kuwahara (1999)	$\rho\varepsilon_\infty$	$\rho\frac{\varepsilon_\infty^2}{k_\infty}$
	$k_\infty=3.7\gamma^{3/2}(1-\gamma)\lvert\mathbf{u}\rvert^2$ $\varepsilon_\infty=39\gamma^2(1-\gamma)^{5/2}\frac{\lvert\mathbf{u}\rvert^3}{d_p}$	
Pedras & de Lemos (2001)	$c_k\rho\frac{k\gamma\lvert\mathbf{u}\rvert}{\sqrt{K}}$ $c_k=0.28$	$c_k\rho\frac{\varepsilon\gamma\lvert\mathbf{u}\rvert}{\sqrt{K}}$ $K=\frac{\gamma^3 d_p^2}{150(1-\gamma)^2}$
Takeda (1994)	$c_k R_0\lvert\mathbf{u}\rvert^2$ $c_k=0.0413$	$c_k R_0\frac{\varepsilon\lvert\mathbf{u}\rvert^2}{k}$

Table 1: Source terms in the turbulence equations for flow through porous media (packing of spheres).

MODEL SET-UP

The base case in the current study is the gas flow through a packed cylindrical column of monosized spheres. The column dimensions are 1.0m long and 0.14m in diameter and the diameter of the inlet/outlet, centrally located, is 0.04m. The sphere diameter is 3mm, and the tube-to-particle ratio is 46.7. The operating condition is based on the work of Paterson et al. (2000). Molecular diffusivity of the tracer gas (CO_2) in air is set to 1.39×10^{-5} m^2/s. We choose this case in order to compare directly with their experimental data.

The local packing structure and resulting porosity variation reflect the wall effect in the numerical model. Typically the radial porosity distribution has a limit of unity at the wall and exhibits an exponential variation combined with a damped oscillation. These fairly well defined radial variations of the porosity are due to the confining effect of the wall of the bed. In a randomly packed bed, the layer of spheres nearest to the wall tends to be highly ordered, with most of the spheres touching the wall at a point contact, and the subsequent layers are less and less ordered, until a fully randomised arrangement is attained far away from the wall. For mathematical convenience, the variation in porosity is fitted by a set of equations (Cohen and Metzer, 1981),

$$\frac{1-\gamma}{1-\gamma_b}=4.5(y-\tfrac{7}{9}y^2),\qquad y\le 0.25$$
$$\frac{\gamma-\gamma_b}{1-\gamma_b}=a_1e^{-a_2y}\cos(a_3y-a_4)\pi,\ 0.25<y<8$$
$$\gamma=\gamma_b,\quad 8\le y<\infty \tag{8}$$

γ_b is the bulk porosity, with a value of 0.35 being used. The constants were determined to be a_1=0.3463, a_2=0.4273, a_3=2.4509 and a_4=2.2011.

SIMULATION PROCEDURE

A commercial CFD code CFX4.4 has been used as a platform, and the porosity and source terms are implemented in the provided user subroutines. The inlet and outlet of the simulation domain are treated as fully developed, and the well-known wall function is used. By fully developed, a distributed velocity profile is solved based on the given flow rate and zero velocity gradient.

In the physical experiment, a pulse of tracer gas is injected from the inlet and is assumed to be fully mixed with the main gas flow before entering the domain. An integral (global) RTD curve is obtained by monitoring the concentration at the exit. In a CFD simulation, the injection of the pulse of tracer is realised by setting a scaler fraction over a short time (in a single time step) on the inlet plane. A two-dimensional axisymmetric simulation is carried out for velocities and turbulence quantities. Then a transient scalar transport is solved, giving a time dependent tracer concentration field. The RTD is obtained by area-averaging the tracer concentration at the outlet for each time step. The Peclet number is defined by the plug flow with axial dispersion model, and is evaluated by fitting an analytical solution to the integral RTD curve predicted.

The time step is chosen to be two orders of magnitude less than the mean residence time in the column. The length scale of the average porosity oscillation is about one particle size. In order to properly implement the oscillatory porosity profile, refined grid spacing must be used near the wall. It is not intended to resolve the flow details below the particle dimension, since we are solving macroscopic flow and the k-ε model was not designed as a sub-grid model as in a large eddy simulation. The grid size used is 200×150. The mass residual for a converged solution is below 1% the total flowrate.

COMPARISON OF THE TURBULENCE MODELS

For simplicity, a section of densely packed bed with uniform porosity is chosen to avoid the complexity of the top and bottom wall effects. A steady fully developed flow with a free-slip wall is simulated, which is equivalent to an infinitely long bed. Except for the molecular diffusion, the effective viscosity calculated is essentially due to the presence of the packing of spheres, since there is no global shear stress present.

The mean effective viscosity (μ_{eff}) averaged over the cross-section is shown in Figure 1, along with the empirical correlation by Bey and Eigenberger (1997). The three models investigated give significantly different results in a wide range of particle Reynolds number (Re_p). The effective viscosity increases with increasing Re_p for all cases, but shows different trends and the order of magnitude. The models of Takeda (1994) and Pedras and de Lemos (2001) generate an eddy viscosity 1-2 orders of magnitude higher than the model of Nakayama and Kuwahara (1999). Parametric study shows that it makes little difference to the result in Figure 1 whether or not the near wall porosity oscillation is considered, and that adjusting c_k does not change the overall trend.

With a fixed Re_p, the effective viscosity predicted by using the model of Nakayama & Kuwahara (1999) is insensitive to the change in particle size, whereas the other two models show strong dependency on particle size (Figure 2). In the latter cases, a lower eddy viscosity corresponds to a larger particle size. According to a review by Pedras and de Lemos (2001), for porous flows in general, the literature recognises that distinct flow regimes are largely determined by the so-called pore Reynolds number, namely: (a) Darcy flow (Re_p<1); (b) Forchheimer flow regime (1~10<Re_p<150); (c) unsteady laminar flow (150<Re_p<300); (d) fully turbulent flow (Re_p>300). This seems to suggest that excessive dependency of μ_{eff}/μ on particle size is not correct. For a flow in a densely packed bed, the turbulence level is controlled mainly by a local equilibrium within the voids between its generation and dissipation, thus the turbulence length scale should be related to particle size. This assumption, for example, leads to an algebraic turbulence model developed by Masuoka and Takatsu (1996) and the one used by Panjkovic et al. (2002), where μ_{eff}/μ is only a function of porosity and Re_p.

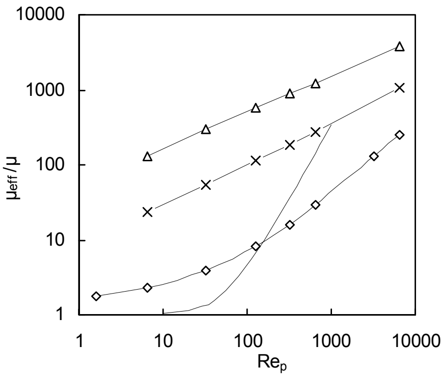

Figure 1: Comparison of the effective viscosity calculated using different turbulence models with experimental correlation: ◇, Nakayama & Kuwahara (1999); △, Takeda (1994); ×, Pedras and de Lemos (2001); full line only, correlation by Bey and Eigenberger (1997).

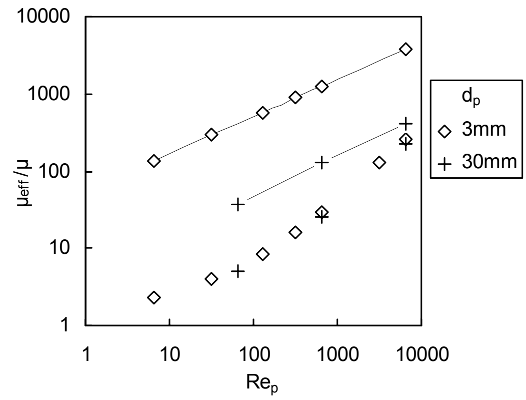

Figure 2: Sensitivity of the effective viscosity to particle size using different turbulence models: symbol only, Nakayama & Kuwahara (1999); full line with symbol, Pedras & de Lemos (2001).

Radially oscillatory behaviour of the velocity distribution has been observed by many investigators. By adjusting an effective viscosity, Bey and Eigenberger (1997) fitted the simulated maximum velocity of the by-pass to the measured values downstream of the bed, and the μ_{eff} obtained was correlated to the Reynolds number in proportion to Re_p^2. This provides qualitative information for the analysis of the present simulation results. For the case of the model by Nakayama and Kuwahara (1999), μ_{eff} increases slowly for low Re_p and becomes nearly proportional to Re_p when Re_p is high. In contrast, the effective viscosity predicted using the other models shows a similar trend, varying in proportion to $Re_p^{0.5}$.

The foregoing discussion suggests that the model by Nakayama and Kuwahara (1999) seems to be superior to the other models considered in terms of giving a realistic trend, thus it is chosen as a standard model in the subsequent simulation. Nakayama et al. (1995) and Kuwahara et al. (1996) showed through numerical experiments that the results based on a two-dimensional numerical model can be used to estimate the pressure drop and thermal dispersion in packed spheres, which further supports our finding.

However, difference in μ_{eff} between the experimental correlation and the prediction using the model by Nakayama and Kuwahara (1999) exists, which may partially be attributed to several reasons. First, the effective viscosity in the model by Bey and Eigenberger (1997) was considered to be constant over the entire bed, while a localised value is more appropriate because of the varying flow conditions. It is found by an observation of the simulation results that the eddy viscosity is relatively low in the centre region and, though oscillatory, increases as approaching the wall, where the higher shear rate (velocity gradient) above the pore scale generates extra turbulence. Second, the accuracy of the model predictions relies to a great extent upon the validity of the available correlations for the porosity profile, since the voidage has a much stronger influence on the velocity profile than the effective viscosity does, as found by Bey and Eigenberger (1997). Finally, the measured velocity profiles a few millimetres downstream of the bed are not necessarily representative of the actual flow field inside the bed.

RESIDENCE TIME DISTRIBUTION

Traditionally the axially dispersed plug-flow model has been used to represent the fluid flow in uniformly packed beds when the diameter of the tubular container is much larger than particle diameter. The mean flow pattern is assumed to be a plug-flow with dispersion caused mainly by mixing of streams in the lee side of particles; the effect of any lateral variations in the interstitial fluid velocity is lumped into a dispersion coefficient. Assuming constant fluid density and dispersion coefficient, D_{ax}, the concentration of a tracer gas in the bed, C(Z,θ), is given by an one-dimensional transport equation (Crawshaw et al., 1993),

$$\frac{\partial C}{\partial \theta}+\frac{\partial C}{\partial Z}=\frac{1}{Pe_l}\frac{\partial^2 C}{\partial Z^2} \tag{9}$$

Pe_l is a Peclet number with the characteristic dimension being the bed length. If the tracer is injected as a Dirac delta function at the bed inlet, the solution to the equation is available for boundary conditions corresponding to an infinitely long packed bed, that is,

$$\frac{\partial C}{\partial Z}=0 \text{ at } Z\to\pm\infty \tag{10}$$

$$C=\delta(\theta) \text{ at Z=0} \tag{11}$$

and is given by Wakao and Kaguei (1982)

$$C(\theta)=\frac{1}{2}\sqrt{\frac{Pe_l}{\pi\theta^3}}\exp\left\{-\frac{Pe_l(1-\theta)^2}{4\theta}\right\} \tag{12}$$

The Peclet number based on particle diameter is,

$$\mathrm{Pe_p}=\frac{ud_p}{D_{ax}}=\mathrm{Pe_l}\frac{d_p}{l} \tag{13}$$

The tracer concentration is normalised to give a comparable RTD in both the experimental measurements and current simulations regardless of the initial tracer concentration,

$$E(t)=\frac{C(t)}{\int_0^\infty C(t')dt'} \tag{14}$$

The mean residence time is calculated as

$$\tau=\frac{\int_0^\infty tC(t)dt}{\int_0^\infty C(t)dt} \tag{15}$$

The tracer is not only carried by the macroscopic mean flow, but can also spread in both lateral and axial direction by means of molecular diffusion/turbulent dispersion. The integral RTD is, therefore, a combined consequence of maldistribution of the velocity due to near wall porosity variation, the effective viscosity and the end effect of the inlet/outlet geometry. Here we use the plug-flow model only for the purpose of easy comparison rather than its validity.

In the RTD simulation, a numerical diffusion due to the truncating error in discretizing the pulse of scalar concentration is not negligible for a low velocity, and in the order of magnitude, it could be as much as the laminar diffusivity. This numerical diffusion acts to broaden the RTD curve. However, the effect of velocity distribution and turbulence becomes dominant as the flowrate increases.

Figure 3 shows the RTD for several conditions: (a) laminar flow with wall effect; (b) turbulent flow without wall effect (uniform porosity to highlight the end effect); (c) turbulent flow with wall effect (normal case). The end effect due to the sudden change in cross-section is important only for a short column. In addition, unlike the volume-averaged macroscopic flow, the actual microscopic fluid moves around the packed spheres in a zigzag path, thus an enhanced scalar mixing is expected even for a low Reynolds number laminar flow. The current turbulence model used is devised for fully turbulent flows. Whether this model could accommodate the mixing effect in the laminar regime in terms of an extended sense of eddy viscosity is a question, but it is evident from Figure 3 that assuming a laminar flow or disregarding the porosity non-uniformity is inappropriate in the simulation, since otherwise a skewed RTD curve could result compared with the measured one. The inclusion of the turbulence model and wall effect does, on the other hand, have improved the prediction of the RTD shape compared with the measured one by Paterson et al. (2000).

An increase of the flowrate (Reynolds number) can change the RTD shape slightly as shown in Figure 4. The RTD for the higher Reynolds number shows an obvious by-pass flow, characterised by a “front tail”. That is, for a higher velocity, the Forchheimer term dominates (the particle shape drag, the second terms in Eq. (5)) over the Darcy term (particle surface friction), which causes a stronger local velocity difference near the wall and subsequently stronger channelling.

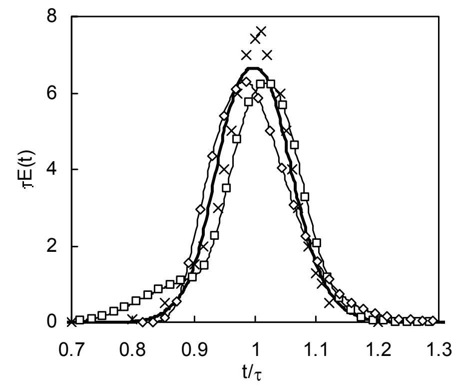

Figure 3: RTD simulated for different assumptions and comparison with measurement (Re_p): □, Laminar with wall effect; ◇, Turbulent without wall effect; thick full line, turbulent with wall effect; ×, measured by Paterson et al. (2000).

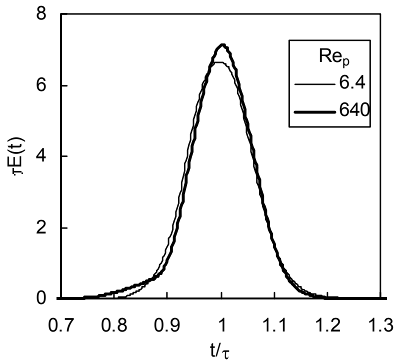

Figure 4: RTD simulated for different Reynolds numbers.

An equivalent value for the Peclet number Pe_p can be obtained by fitting the plug model Eq. (13) to the predicted RTD curves by the least-square method. Figure 5 shows the predicted Pe_p as Re_p changes (by changing the gas flowrate and fixing Sc=0.95), together with some experimental data reported in the literature (Wen and Fan, 1975; Crawshaw et al., 1993). A correlation for the Peclet number was given by Wen and Fan (1975) as,

$$\frac{1}{Pe_p} = \frac{0.3}{ScRe_p} + \frac{0.5}{1 + \dfrac{3.8}{ScRe_p}} \tag{16}$$

The simulated Pe_p agrees closely with the correlation of Wen and Fan (1975) over a wide range of $ScRe_p$ above 60, indicating that the current numerical model performs well for the fixed bed. In view of the numerical diffusion and the discrepancy between the available experimental data for low Reynolds numbers, the difference is still acceptable. It can be seen from Figure 5 that the Peclet number approaches a constant as Re_p increases above 1000, implying that the axial dispersion coefficient, like the effective viscosity, is proportional to particle size and mean gas velocity for high Reynolds number flows.

Since the resistance force is closely related to porosity, the radial variation of the velocity (Figure 6) basically follows the porosity profile except at the wall boundary where no-slip is imposed. The effect of the eddy viscosity on the velocity profile is relatively unimportant compared with the body force.

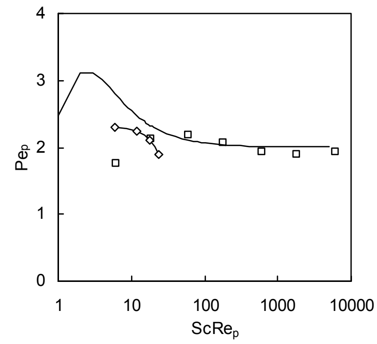

Figure 5: Peclet number for different particle Reynolds numbers: full line only, correlation of Wen and Fan (1975); □, Current simulation; ◇, Crawshaw et al. (1993).

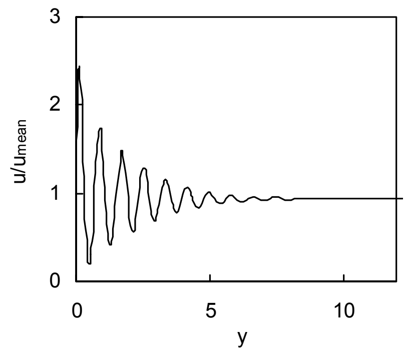

Figure 6: Radial distribution of velocity simulated.

Although the oscillatory nature of the velocity has been observed downstream of the packed bed by many authors (Bey and Eigenberger, 1997; Subagyo et al., 1998), accurate measurement inside the bed is difficult. Paterson et al. (2000) tried to measure the local velocity indirectly by the tracer method. They injected a pulse of tracer gas at a radial location and monitored the concentration 0.5m downstream at exactly the same radial location. By the same way in the simulation, we found that the local mean residence time does not show any oscillation with radius, and the velocity thus obtained increases consistently towards the wall (Figure 7). While the tracer can spread through molecular diffusivity, turbulence further enhances the radial mass transfer at the near wall region. The simulated velocity distribution appears to be consistent with that of Paterson et al. (2000), except at the immediate proximity to the wall (within $2d_p$), where the measured velocity shows a relatively stable value. Nevertheless, it is clear from the simulation that the mean residence time alone does not fully represent the true local velocity and that the velocity profile calculated based on the tracer method without considering the radial mixing may be misleading. The current CFD model is able to repeat many observed phenomena.

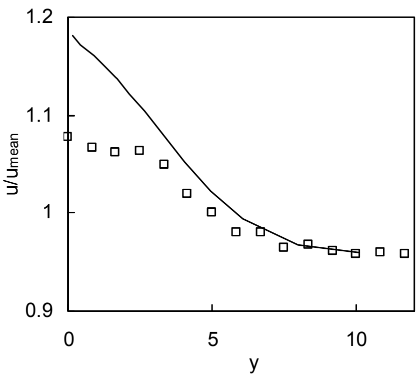

Figure 7: Radial distribution of velocity using tracer method: full line, current; □, measured by Paterson et al. (2000).

CONCLUSIONS

Several turbulence models for porous flows have been applied to the gas flow in a circular packed column of spheres and validated against each other and against experimental data in literature. These models perform rather differently, with the model by Nakayama & Kuwahara (1999) giving the most reasonable eddy viscosity. The chosen turbulence model is able to account for the mixing and mass transfer within the bed. By considering the local porosity variation near the wall, the basic features of the velocity distribution and the RTD predicted are consistent with those measured. The predicted Peclet numbers defined by the plug flow model are close to the experimental results.

The current work shows that the chosen turbulence model is suitable for simulating the flow in porous media of spheres, particularly at high Reynolds numbers. The numerical model is potentially useful to such applications as packed beds in general. Future work will further validate the current turbulence model coupled with heat transfer.

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