2-D MATHEMATICAL AND NUMERICAL MODELINGS OF FLUID FLOW INSIDE AND OUTSIDE PACKING IN CATALYTIC PACKED BED REACTOR

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ABSTRACT

Generally, the momentum equation of fluid flow in porous media was solved by neglecting the terms of diffusion and convection such as Ergun, Darcy, Brinkman and Forchheimer models. Their models primarily applied for laminar flow. It is true that these models are limited to conditions whether the models can be applied. Analytical solution for the model types above is available only for simple one-dimensional cases. For two or three-dimensional problem, numerical solution is the only solution. This work advances the flow model in porous media and provides two-dimensional flow field solution in porous media, which includes the diffusion and convection terms. The momentum lost due to flow and porous material interaction is modeled using the available Brinkman-Forchheimer equation. The numerical method to be used is finite volume method. This method is suitable for the characteristic of fluid flow in porous media which is averaged by a volume base. The effect of the solid and fluid interaction in porous media is the basic principle of the flow model in porous media. The Brinkman-Forchheimer model considers the momentum loss term to be determined by a quadratic function of the velocity component. The momentum and continuity equations are solved for two-dimensional cylindrical coordinate. The results were validated with the experimental data. The porosity of the porous media was treated to be radially oscillated. The results of velocity profile inside packing show a good agreement in their trend with the Stephenson and Stewart experimental data. The local superficial velocity attains its global maximum and minimum at distances near 0.201 and 0.57 particle diameter, d_p. Velocity profile below packing was simulated. The results were validated with Schwartz and Smith experimental data. The results also show an excellent agreement with those experimental data.

Keyword: finite volume method, porous media, flow distribution, velocity profile

INTRODUCTION

Catalytic packed bed reactor is the type reactor that's widely used in many chemical industries. The reactor is packed with porous catalyst particle. In catalytic packed bed reactor, the fluid flow phenomena is very complex because the fluid will pass porous media therefore fluid flow in porous media must be really considered. The mechanism of the flow in porous media involves many problems vital to science and industry. Notable examples are chemical catalytic reactors, chemical adsorption column, filtration, chemical membrane separation, reservoir engineering, biomechanics, geophysics, hydraulics, soil mechanics and others.

The phenomena of flow distribution in packed bed have been formulated through several experiments. The measurement of flow inside packing has been done by McGreavy, *et. al*, (1986) and Stephenson and Stewart (1986). McGreavy, *et. al* using Doppler-laser anemometer while Stephenson and Stewart using a marker tracing method to observe the fluid motion with a video camera in a transparent packed bed. It was found that the local superficial velocity attained its global maximum and minimum at distance near 0.2 d_p and 0.5 d_p from the wall. McGreavy obtained the maximum velocity at 0.3 d_p from the wall. The other researchers such as Morales, *et. al*, (1951), Schwartz and Smith (1953), Schertz and Bischoff (1969), Marivoet, *et. al*, (1973) and Lerou and Froment (1976) measured velocity profile at region above or below packing at distance about one to three times particle diameter. The flow distribution was given by fluid velocity measurement which was carried out

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using hot-wire anemometer (HWA) or Laser-Doppler-Anemometer (LDA). The experimental results show the flow characteristics drastically change when flow leaves packing. This indicates the measurement of fluid velocity obtained exit packing is not fully representing real flow information inside the bed.

Mathematical modelings of fluid flow in porous media have been widely developed. Among of them are models that are developed by Darcy (1856), Brinkman (1949), Forchheimer (1901) and Ergun (1952). The models are applied specifically to laminar flow. However, those models are limited to one-dimensional flow and historically obtained through empirical approach. The original mathematical forms of the models absurd have not yet describe the complete components of momentum transfer. Some author extended directly one-dimensional models above to two and three-dimensional models. Two-dimensional numerical investigation was developed by Stanek and Szekeley (1974) and Papageorgiu and Froment (1995). The momentum equations were simplified into two-dimensional mathematical model that correlate the pressure gradient and velocity component. The unknown pressure field was handled by transforming the equations into vorticity transfer equation. The solution was obtained numerically using finite difference method. The mathematical model solutions are limited up to two-dimensional problem. However, the vorticity method used Stanek and Szekely (1974) and Papageorgiu and Froment (1995) is not so much reliable method due to its limitation to two-dimensional laminar problem only.

The numerical and computational developments have been established by Buchori, *et al.* (2000). The finite volume method is used to obtain the solution. The effects of particle sizes and Reynold number were reported in his previous work. In this research, the mathematical model for the momentum equation of flow in porous media is developed. The Brinkman-Forchheimer equation is adopted to model the effect of fluid and solid interaction giving the momentum loss to the flow field equation. Velocity profile inside and outside packing reactor were simulated. The results were validated with the experimental data. Beside the mathematical model development, the more general solution method of flow adopted for the preparation to extend the solution method for three-dimensional flows.

CHARACTERISTIC OF POROUS MEDIA

The characteristic of flow in porous media depend on properties and structure of itself. There are two important parameters to differentiate between the porous and empty media. The ratio between pore volume (fluid volume) and continuum medium volume (solid and fluid volumes) quantifies the space, which can be flown by the fluid. This ratio is recognized as porosity, ε. The other parameter for the fluid flow in porous media is tortuosity, τ. Tortuosity is the ratio between the global passage distance of the flow in a continuum volume (macroscopic distance) and that total passage distance of the flow in pore network straits (microscopic distance) in a continuum volume.

The porosity is a quantitative that describes the fraction of the voids medium. In experiments have been done by researchers such as Roblee, *et. al* (1958), Benenati and Brosilow (1962), Ridgway and Tarbuck (1966), Thadani and Peebles (1966), Pillai (1977), Schuster and Vortmeyer (1980), porosity in packed bed is not uniform. Porosity at reactor wall is higher than bulk. The results show that maximum value of porosity is attained at wall with ε = 1. The porosity will be decreased and will attain constant value at fixed distance from wall. However, this decreased not linier but oscillated along reactor radius until distance 3 – 5 particle diameter.

The researchers made model to illustrate porosity profile along radial direction (Martin, 1978; Cohen and Metzner, 1981; Vortmeyer and Schuster, 1983; Mueller, 1990; Liu and Masliyah, 1999). This research using Liu and Masliyah model (1999) because their model is a better fit to the experimental data for packed beds of uniform spheres and cylinders. Their model is,

$$\varepsilon = \varepsilon_b + \left(1-\varepsilon_b\right)Er * \left[\left(1-0.3p_d\right)\cos\left(\frac{2\pi}{1+1.6Er^2}\,\frac{D/2-r}{p_d d_s}\right)+0.3p_d\right] \quad (1)$$

The exponential decaying function is given by

$$Er = \exp\left[-1.2p_d\left(\frac{D/2-r}{d_s}\right)^{3/4}\right] \quad (2)$$

For packed bed of uniform spheres, the period of oscillation is, $p_d = 0.94$

MATHEMATICAL MODELING IN CATALYTIC PACKED BED REACTOR

An ideal approach to establish the fluid flow model inside porous media is to define the momentum and continuity equations inside pore volumes only and treat the solid media as zero boundary for the flow field. However, this approach is not practical and very tedious. The most common approach is to assume the whole porous media (solid and pore volume) as a continuum medium. The flow governing equations work on this continuum medium without considering whether solid or fluid medium. All quantities are defined on the bases of volume average.

A local quantity Φ^{ℓ} is used to define a volume average quantity Φ. This called is REV (*Representative Elementary Volume*) (Slattery, 1969; Liu and Masliyah, 1999). The volume average of a point quantity associated with the fluid quantities (velocity, density, concentration or other) is

$$\Phi = \frac{1}{\Delta\upsilon}\int \Phi^{\ell} d\upsilon \qquad (3)$$

So that, the continuity equation for porous media is written in a control volume average, $\Delta\upsilon$,

$$\frac{1}{\Delta\upsilon}\int \frac{\partial}{\partial t}(\varepsilon\rho)d\upsilon + \frac{1}{\Delta\upsilon}\int(\rho\vartheta_i)d\upsilon = 0 \qquad (4)$$

That equation can be written,

$$\frac{\partial\rho}{\partial t} + \frac{1}{\varepsilon}(\nabla \bullet \rho\vartheta_i) = 0 \qquad (5)$$

The general momentum equations of fluid flow in porous media in a control volume υ constitute rate of increase of momentum, rate of momentum gain by convection, rate of momentum gain by viscous transfer (diffusion), pressure force, gravitational force or external force, and rate of momentum loss due to fluid and solid interaction in porous media. The momentum equations in porous media are averaged in a control volume as the following

$$\frac{1}{\Delta\upsilon}\int \frac{\partial}{\partial t}(\varepsilon\rho\bar{\vartheta}_i)d\upsilon + \frac{1}{\Delta\upsilon}\int(\rho\bar{\vartheta}_i\vartheta_j)d\upsilon = \frac{1}{\Delta\upsilon}\int \varepsilon\rho f\, d\upsilon + \frac{1}{\Delta\upsilon}\int \varepsilon(\tau_{ij})_j d\upsilon - \frac{1}{\Delta\upsilon}\int \varepsilon\nabla P\, d\upsilon \qquad (6)$$

The averaged volume viscous term, the second term in the right hand side of Eq. (6), should be very complex to be derived resulting a well defined term. This term can be contributed also the momentum loss due to the fluid and solid interaction. Intuitively, the viscous term is defined by the diffusion rate of momentum and the new term for momentum loss due to the fluid and solid interaction is added to Eq. (6), specific flow models are resulted. The fluid and solid interaction term is model by Brinkman-Forchheimer equation. At last, specific flow model is obtained as the following

$$\frac{\partial}{\partial t}(\rho\vartheta_i) + \frac{1}{\langle\varepsilon\rangle}\frac{\partial}{\partial x_j}(\rho\vartheta_i\vartheta_j) = \rho g_i + \frac{\partial}{\partial x_j}\left(\mu\frac{\partial\vartheta_i}{\partial x_j}\right) - \frac{\partial P}{\partial x_i} - \frac{\mu}{k}\vartheta_i - \beta\rho\vartheta_i\vartheta_i \qquad (7)$$

NUMERICAL MODELING AND COMPUTATIONAL METHOD

Momentum equations of fluid flow in porous media were modeled in the past using laminar Darcy, Brinkman, Forchheimer, Ergun, modified Ergun flows. Those models neglect diffusion and convection terms except Brinkman model added intuitively the diffusion term only and still neglect the convection term. As a consequence the effect of convection term to flow distribution is not observed

In this work research, the porous media flow is modeled by including the convection and the diffusion terms. Brinkman-Forchheimer model is adopted to model the momentum loss due to fluid and solid interaction which appears as an additional term in the momentum equation as is shown in Eq. (7). A specific mathematical modeling of fluid flows in porous Equation, Eq. (7), improves conventional models in term of the present of both convection and diffusion terms. Furthermore, this model can be developed to a numerical model.

A numerical modeling of fluid flow in the porous media is developed from Eq. (7). The momentum, Eq. (7) and continuity, Eq. (5), are presented for steady state and two-dimensional cylindrical coordinate. The flow is incompressible and isothermal. The flow in porous media is limited to Forchheimer flow. This results two-dimensional continuity equation,

$$\frac{1}{\varepsilon}\frac{\partial}{\partial z}(\rho u) + \frac{1}{\varepsilon}\frac{1}{r}\frac{\partial}{\partial r}(\rho v r) = 0 \qquad (8)$$

and two dimensional momentum equations written in the form of flux variables J, source term S and pressure gradient

$$\frac{\partial}{\partial z}(J_{\vartheta z}) + \frac{1}{r}\frac{\partial}{\partial r}(rJ_{\vartheta r}) = -\frac{\partial P}{\partial x_i} + S_{\vartheta} \qquad (9)$$

where

$$J_{\vartheta z} = \left(\frac{1}{\varepsilon}\rho\vartheta_i\vartheta_j - \mu\frac{\partial\vartheta_i}{\partial z}\right) \qquad (10)$$

$$J_{\vartheta r} = \left(\frac{1}{\varepsilon}\rho\vartheta_i\vartheta_j - \mu\frac{\partial\vartheta_i}{\partial r}\right) \qquad (11)$$

$$S_{\vartheta} = -\frac{\mu}{k}\vartheta_i - \beta\rho\vartheta_i^2 \tag{12}$$

Equations (9) to (12) are closure forms and numerically solvable. Well known finite volume method Patankar (1980) is used in to model numerically Eq. (8) to (12). The computational domain is defined as the duct geometry of the flow to form a continuum volume. Subsequently, this computational domain is discretized in finite control volumes. Conservation laws must be valid at each control volume and so the whole computational domain. The discretization of momentum and continuity equations forms a set of linear algebraic equation. This set of linear algebraic equations is solved iteratively using a line-by-line method matrix solver. For each line, linear algebraic equations are solved using tridiagonal matrix direct solver, TDMA (Tridiagonal Matrix Algorithm). Unknown pressure field is handled using a standard SIMPLE procedure.

The source term, Eq. (12), is linearized in the form of

$$S = S_C + S_P\vartheta_P \tag{13}$$

The coefficient S_p is kept always less than or equal to zero. To meet with this criterion, this source is linearized following

$$S = S^{*} + \left(\frac{dS}{d\vartheta}\right)^{*}\left(\vartheta_P - \vartheta_P^{*}\right) \tag{14}$$

The symbol ϑ_P^{*} is used to denote the previous-iteration value of ϑ_P.

RESULTS AND DISCUSSION

The computational parameters were set to be the same as experimental parameters of Stephenson and Stewart (1986). The pipe diameter D, particle diameter d_p, particle Reynold number Re_p, tube length L, bulk porosity ε_b are respectively 75.7 mm, 7.035 mm, 280, 144.9 mm, 0.354. Experimental measurement of axial velocity was measured by averaging at distance 0.05 of pipe radius R. The grid size in the computation was set also to the length of 0.05 R. The porosity of the bed follows the profile of Eq. (1).

The results of flow field velocity computation in packed bed catalytic reactor are compared to measured axial velocity profile given by Stephenson and Stewart (1986), which used optical measurement technique. Reactor configuration in this research is shown in Fig. 1. The axial velocity component profile is shown in Fig. 2 and the radial is presented by Fig. 3. The vector of these velocity components is depicted in Fig. 4.

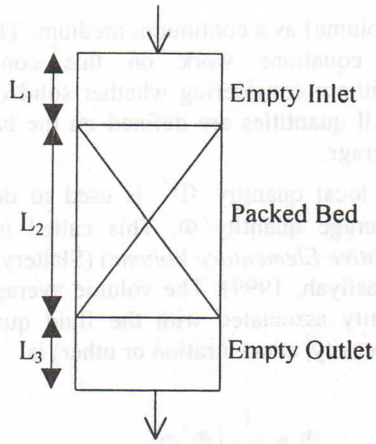

Figure 1. Reactor configuration

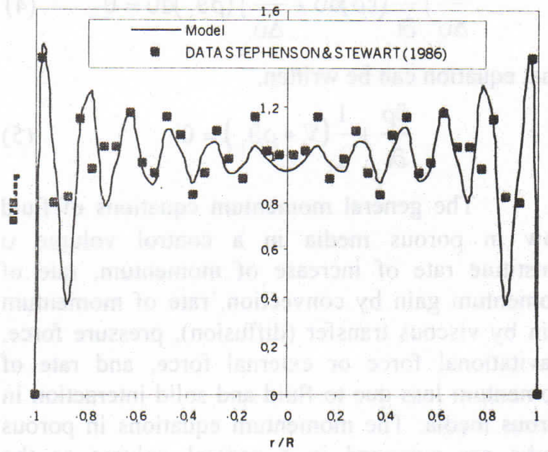

Figure 2. Axial velocity profiles inside packed bed reactor (L_2)

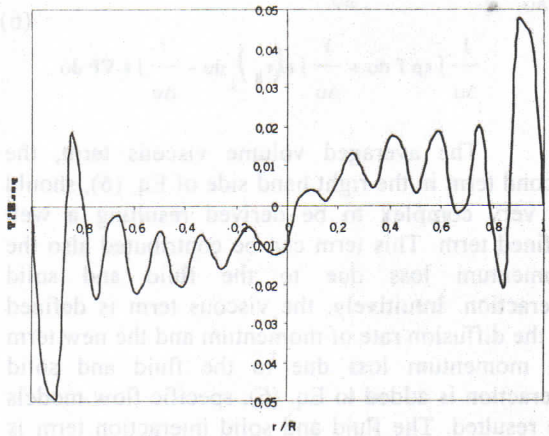

Figure 3. Radial velocity profile inside packed bed reactor (L_2)

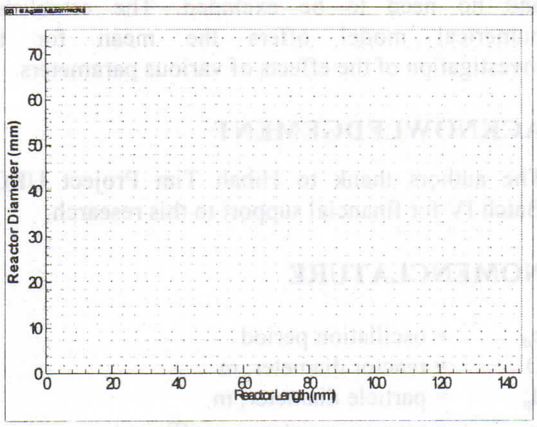

Figure 4. Profile of velocity along the inside packed bed reactor (L_2)

Those figures indicate that velocity profile produce the trend of having global maximum and minimum peaks at distance very close to the wall. The predicted flow fields agree closely to measured velocity from Stephenson and Stewart's experiment.

In accordance with Staphenson and Stewart, the first maximum and minimum peak should occur at distance 0.2 d_p and 0.5 d_p from the wall. This value becomes a critical criterion in comparing the predicted results using various models and experimental results (Cheng and Yuan, 1997). These computational results give the first maximum peak at distance 0.201 d_p and the first minimum peak at 0.57 d_p. This means that in term of the quantity, these computational results are quite accurate.

A quasi-analytical solution for one dimensional at those experimental parameters above was obtained by Cheng and Yuan (1997). Their results indicate the second maximum peak to occur at 1.0 d_p from the wall. The second peak from the present results occurs at distance 1.07 d_p, that is almost the same value as Cheng and Yuan result above.

The comparison of present numerical modeling results with experimental and quasi-analytical results leads to some important findings. The convection and the diffusion terms in the mathematical modeling can be solved numerically and no need to be excluded. The effect of these terms to the flow field prediction exists especially to complex flow configuration that can be solved one-dimensional approach. It may be argued that these terms can be neglected. This practice may be valid for strong one-dimensional flow in porous media. This numerical model is considered to be accurate. Furthermore, the radial velocity profile can be predicted in which its importance is very clear for real flow, non one-dimensional flow. There are various non-ideal problems of the flow in porous media can be investigated using this numerical model.

Furthermore, the computational program is solved to investigate velocity distribution at region below packing. The computational parameters were set to be the same as experimental parameters of Schwartz and Smith (1953). Schwartz and Smith experiment is conducted by change reactor diameter and particle packing. The reactor diameter used is 2, 3 and 4 in. The size particle packing is ¼ and 3/8 in. The form of particle packing is a uniform cylinder equilateral. The fluid, tube length L, bulk porosity ε_b are air, 23 in, 0.32 respectively. The results are shown in Fig. 5, 6 and 7.

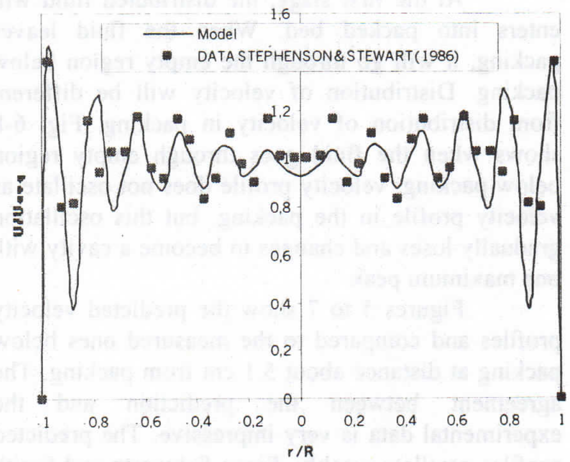

Figure 5. Velocity profile at distance 5.1 cm below packing (D=2 in, dp=1/4 in) (L_3)

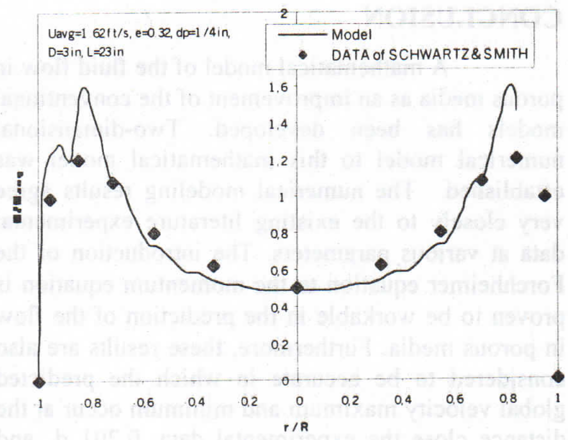

Figure 6. Velocity profile at distance 5.1 cm below packing (D=3 in, dp=1/4 in) (L_3)

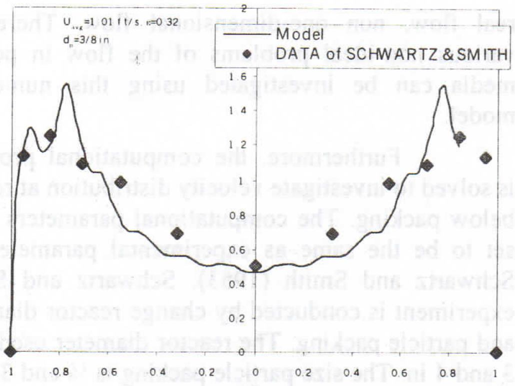

Figure 7. Velocity profile at distance 5.1 cm below packing (D=4 in, dp=3/8 in) (L_3)

At the first stage, the distributed fluid will enters into packed bed. When the fluid leaves packing, it will go through the empty region below packing. Distribution of velocity will be different from distribution of velocity in packing. Fig. 6-8 shows when the fluid goes through empty region below packing, velocity profile does not oscillate as velocity profile in the packing, but this oscillation gradually loses and changes to become a cavity with one maximum peak.

Figures 5 to 7 show the predicted velocity profiles and compared to the measured ones below packing at distance about 5.1 cm from packing. The agreement between the prediction and the experimental data is very impressive. The predicted profiles oscillate weakly. Since Schwartz and Smith (1953) took only five experimental points, the presence of oscillation in measured velocity was not captured.

CONCLUSION

A mathematical model of the fluid flow in porous media as an improvement of the conventional models has been developed. Two-dimensional numerical model to this mathematical model was established. The numerical modeling results agree very closely to the existing literature experimental data at various parameters. The introduction of the Forchheimer equation to the momentum equation is proven to be workable in the prediction of the flow in porous media. Furthermore, these results are also considered to be accurate in which the predicted global velocity maximum and minimum occur at the distance close the experimental data, 0.201 d_p and 0.57 d_p. The computational results also indicate a good agreement with experimental data when it is simulated at region below packing. Thus, the convection and the diffusion terms in the mathematical modeling can be solved numerically and no need to be excluded. The established numerical model offers the mean for the investigation of the effects of various parameters.

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NOMENCLATURE

p_d = oscillation period
D = reactor diameter, m
d_p = particle diameter, m
α = viscous resistance coefficient
β = inertia resistance coefficient
ε_b = bulk porosity
G = gravitation force, m/s^2
Er = exponential decaying function
k = permeability, m^{-2}
L = packing length, m
S = source term
p = pressure, $kg/m.s^2$
Re_p particle Reynold number
r = reactor radius, m
u = superficial velocity x-direction, m/s
v = superficial velocity y-direction, m/s
ε = porosity
μ = fluid viscosity , kg/m.s
ρ = fluid density, kg/m^3
ρu_i = mass flux, $kg/m^2.s$
$\rho u_i u_j$ = momentum flux, $kg/m.s^2$
∇ = nabla, operator gradient
J = flux
Subscript: 0 = initial value

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