Utilizing Shear Factor Model and Adding Viscosity Term in Improving a Two-Dimensional Model of Fluid Flow in Non Uniform Porous Media

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Abstract. In a packed bed catalytic reactor, the fluid flow phenomena are very complicated because the fluid and solid particle interactions dissipate the energy. The governing equations were developed in the forms of specific models. The shear factor model was introduced in the momentum equation for covering the effect of flow and solid interactions in porous media. A two dimensional numerical solution for this kind of flow has been constructed using the finite volume method. The porous media porosity was treated as non-uniform distribution in the radial direction. Experimentally, the axial velocity profiles produce the trend of having global maximum and minimum peaks at distance very close to the wall. This trend is also accurately picked up by the numerical result. A more comprehensive shear factor formulation results a better velocity prediction than other correlations do. Our derivation on the presence of porous media leads to an additional viscosity term. The effect of this additional viscosity term was investigated numerically. It is found that the additional viscosity term improves the velocity prediction for the case of higher ratio between tube and particle diameters.

Keywords: *effective viscosity; flow fluid; non-uniform porous media; numerical modeling; shear factor.*

1 Introduction

Catalytic packed bed reactor is the type of reactor that is widely used in many chemical industries. The reactor is packed with porous catalyst particles. A flow distribution problem occurs frequently in the operation of packed bed reactor. The problem is often referred to flow mal-distribution. Generally, the flow mal-distribution is caused by inherent reactor design and operation problems, which

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fail to meet the required flow distribution. At present, a reactor is designed mostly using the simplification method of flow in which the complicated flow that may exist is assumed to be simple and has known flow characteristics, such as resulting elementary reactor design procedures either perfectly mixed or plug flow reactor design concept. An improved reactor design method should be observed. If the flow field can be predicted realistically, the flow mal-distribution can be minimized or avoided by the geometry modification in the design step. In catalytic packed bed reactor, the fluid flow phenomena are very complicated because there is an interaction between the fluid flow and solid particles/porous medium. The interaction will dissipate the energy of flowing fluid.

Mathematical and numerical modelings for prediction of fluid flow field in porous media have been widely developed. Giese, et al. [1] and Liu and Masliyah [2] have solved one-dimensional problem by neglecting convection terms and using finite difference method. Stanek and Szekely [3] and Papageorgiou and Froment [4] solved the two-dimensional problem using vorticity method. Their solution is not much reliable due to its limitation to two-dimensional laminar problems only. The mathematical and numerical models are needed to be developed to obtain a more realistic solution of fluid flow field in porous media. The model and method should be flexible in variation of porous media properties, expandable to three-dimensional model, and ready to incorporate mass and heat transfers.

The treatment of porous media in the past was carried out by most authors with constant porosity. The calculated velocity profiles were considered as a velocity profile in a fluid like region. However, this work used a non-uniform porosity approach of the media. This is because of that the real condition of the media porosity is not uniform. The porosity profile is obtained from the measurement data by Benenati and Brosilow [5]. The computed velocity profiles should become more realistic in which the velocity in the region with higher porosity should be higher than the velocity in the region with lower porosity.

The effect on this expected velocity distribution will be more prompt to the reaction process in the porous media. If the computed velocity is based on uniform porosity approach, the predicted chemical component concentration profile will be considered not to represent the actual condition. This work focused on the computational method and fluid flow physical models for non uniform porous media. When velocity distributions are well predicted numerically, the chemical reactions can be easily included to be computed together with velocity components by adding their mass conservation equations.

The momentum equations for porous media are different from that for full fluid media in the term of the additional friction term. The friction in porous media was originally formulated from experimental data to state the relation between the pressure drop and the superficial velocity of the fluid. The earlier correlations are based on the absence of the convection contribution to the momentum equations like Darcy's, Forcheimer and Brinkman equations. The later correlations were constructed from experiments. These friction correlations are given in Table 1.

For two dimensional flow, the momentum equations are constructed by convection, diffusion, and friction terms. The definition of the friction term in this work is adopted from the relation between the pressure drop and the fluid velocity described above. The x-momentum equation uses the same construction of the friction relation with the y-momentum equation except its velocity variable in the friction equation in which it uses its own velocity direction.

Many expressions of the friction equation are available. The clarification on which friction term expression to provide a good prediction in velocity profiles needs to be investigated. The contribution of this work is on filling the information gap on this matter.

Liu and Masyliah [2] considered the effect of porous media in enhancing the diffusional momentum term. The conventional approach does not have this additional diffusional term in the momentum equation. Their postulation is a kind of complex formulation. It is our interest to simplify this complex formulation to a simple one. Our simplified formula was derived to form an additional viscosity to give an effective viscosity in the diffusional term of the momentum equations. Therefore, this can be easily studied numerically to investigate this postulation in a more simple way.

The objectives of this research are (i) to construct a numerical solution to solve two-dimensional continuity and momentum equations for the fluid flow in non-uniform porous media which involves various shear factor expressions, (ii) to investigate which shear factor expression can give a better prediction of the velocity field, (iii) to form a simplified formula of the additional contribution by porous media to the momentum transfer and (iv) to investigate numerically the additional contribution by the porous media to the momentum transfer. Specific models of flow in porous media have been derived in which these models are more comprehensive in considering two-dimensional case covering diffusion, convection, and shear factor terms. The numerical procedures and solution have been established.

The measurement of the velocity components inside the porous media is not easy. It requires a complicated and advanced technique. For the purpose of this study, the available experimental data from literatures we used. There are two sets of experimental data available. The first set is the experimental data of Kufner and Hofmann [6] and the second is the data of Stephenson and Stewart [7]. These data are very useful for this study. First, the numerical predictions show the trend of the superficial velocity field in a good agreement with and Stephenson and Stewart [7]. By comparing to the experimental data, Liu and Masliyah shear factor correlation results a better velocity production than other correlations do. The existence of the porous media was derived to contribute on an additional viscosity. The effect of this additional viscosity was successfully investigated numerically [8]. It is found that the additional viscosity improves the velocity prediction for the case of higher ratio between tube and particle diameters.

2 Mathematical Modeling of Fluid Flow in Porous Media

Fluid flow field in porous media can be obtained by solving the momentum, continuity, and species concentration transfer equations simultaneously. For the interest of fluid flow only in which the mass transfer is not involved, the momentum and continuity equations govern this phenomenon. The momentum and continuity equations in porous media should be derived to cover the effect of solid porous media to the fluid flow.

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 to treat the solid media as zero boundaries 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 base of volume average.

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 known as porosity, ε. Another parameter of 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 the continuum volume.

A local quantity Φ^{ℓ} is used to define a volume average quantity Φ. If a control volume is Δ_V, a volume average of quantity is defined by Stanek and Szekely [3] as

$$\Phi = \frac{1}{\Delta_V}\int \Phi^{\ell} dV \tag{1}$$

Volume average quantities for fluid flow field are usually referred as superficial velocities. Consequently, the superficial velocities are also spatially distributed. Spatial distribution of superficial velocities provides the information of fluid velocity field. Other quantities, such as fluid and solid properties, are also presented as volume average quantities.

The continuity equation of fluid flow in porous media can be averaged in a continuum control volume,

$$\frac{1}{\Delta_V}\int \frac{\partial}{\partial t}(\varepsilon\rho)\, dV + \frac{1}{\Delta_V}\int (\nabla \bullet \rho\vartheta_i)\, dV = 0 \tag{2}$$

Equation (2) is finalized in the form of

$$\frac{\partial \rho}{\partial t} + \frac{1}{\varepsilon}(\nabla \bullet \rho\vartheta_i) = 0 \tag{3}$$

At steady state condition and two-dimensional directions, axial and radial, Equation (3) leads to

$$\frac{1}{\varepsilon}\frac{\partial}{\partial z}(\rho u) + \frac{1}{\varepsilon}\frac{1}{r}\frac{\partial}{\partial r}(r\rho v) = 0 \tag{4}$$

The general momentum equations of fluid flow in porous media in a control volume Δ_V constitute rate of increase of momentum, rate of momentum gained by convection, rate of momentum gained by viscous transfer (diffusion), pressure force, and gravitational force or external force. Each of these terms can be averaged in a control volume of continuum medium. The averaged flux (total convection and diffusion) can be composed mathematically in a transfer quantity inside the control volume, the transfer quantity between fluid and solid media.

Based on the volume average above, Liu and Masliyah [2] derived the momentum equations of flow in porous media to give more general equations as follows:

$$\frac{\partial}{\partial t}\frac{\rho\vartheta_i}{\tau}+\nabla\bullet\left(\frac{\rho\vartheta_i\vartheta_j}{\varepsilon\tau}\right)=$$
$$\nabla\bullet\tau\mu\left[\nabla\vartheta_i+\left(\nabla\vartheta_j\right)^T\right]+\nabla\bullet\left(\tau\varepsilon\underline{\underline{K}}\bullet\nabla\frac{\rho\vartheta_i}{\tau\varepsilon}\right)-\tau\ \nabla p-\rho g\ +\tau\mu F\vartheta_i \tag{5}$$

One can overview the momentum equations above as mathematical modeling equations for fluid flow in porous media. The second term in the right hand side of Equation (5) was a postulated closure form as an extra term for interaction flux within the fluid, which can be simplified into a similar form to diffusion. The first term in the right hand side of Equation (5) is a pure diffusion term. Both of these terms can be combined to give a total diffusion term.

The quantity $\underline{\underline{K}}$ was defined as a tensor of dispersion coefficients by Liu and Masliyah [2],

$$\underline{\underline{K}}=d_p\left|\vartheta_i\right|D_T\begin{vmatrix}\delta_L & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{vmatrix} \tag{6}$$

Where d_p, D_T and δ_L are particle diameter, transverse dispersion coefficient and normalized longitudinal dispersion factor respectively.

The last term in the right hand side of Equation (5) represents the total flux from fluid to solid. Moreover, the form used by these authors was a specific proposed model for flux exchange between fluid and solid. The factor F was termed as the shear factor and considered to be a function of its local Reynolds number. The shear factor in a momentum transfer indicates the momentum loss due to fluid and solid interaction.

For the moment, Equation (5) is the most comprehensive momentum equation for fluid flow in porous media. This equation will be used to form a more specific mathematical model of fluid flow in porous media which will be evaluated in this work. Further simplification of Equation (5) can lead to conventional mathematical models of flow in porous media, such as Darcy's, Brinkmam's, and Forchheimer's equations**.**

The diffusion contribution to a momentum transfer is determined by a diffusion coefficient. The diffusion coefficient for the laminar flow in full fluid duct is a dynamic fluid viscosity. For the turbulent flow, the total diffusion coefficient is obtained by adding the turbulent viscosity or eddy viscosity to the dynamic fluid viscosity. For the flow in the porous media, the solid porous media contribute to enhance the uniformity of the flow distribution. The use of dynamic fluid viscosity only for the flow in the porous media does not follow this logical concept. For this reason, the diffusion coefficient for the fluid flow in the porous media can be established by taking an analogical approach to the turbulent flow to give an effective viscosity μ_{eff} as the following,

$$\mu_{eff} = \mu + \mu_p \tag{7}$$

Variable μ is the dynamic viscosity of the fluid and μ_p is the porous viscosity (diffusion coefficient) contributed by the presence of the solid matrix in a continuum medium.

Two fundamental reasons can be built to support the concept of increasing viscosity by the porous media, Equation (7). First, the solid medium actually diffuses through the fluid flow leading to a flatter velocity gradient. A flatter velocity gradient in momentum transfer is produced by higher viscosity. This phenomenon is shown by Equation (7). Second, the first two terms in the right hand side of Equation (5) represent the diffusion momentum transfer. The dispersion coefficient tensor K for x-direction has components K_{xx}, K_{yx} and K_{zx}.

A three-dimensional Cartesian coordinate as an x-momentum component expresses the two diffusion terms above,

$$\nabla \bullet \left[\tau\mu \left(\nabla \vartheta_i + \nabla \vartheta_i^T \right) \right] + \nabla \bullet \left(\tau\varepsilon \underline{\underline{K}} \bullet \nabla \frac{\rho \vartheta_i}{\tau\varepsilon} \right) =$$

$$\frac{\partial}{\partial x}\left[\tau(\mu+\rho K_{xx}) \frac{\partial u}{\partial x} \right] + \frac{\partial}{\partial y}\left(\tau(\mu+\rho K_{yx}) \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial z}\left[\tau(\mu+\rho K_{zx}) \frac{\partial u}{\partial z} \right] \tag{8}$$

$$\mu_{eff} = \mu + \rho K \tag{9}$$

The total diffusion coefficient in Equation (8) is obtained to give a similar form to Equation (6). As the result, the effective viscosity concept for a fluid flow in porous media is proposed logically, Equation (7), and theoretically, Equation (9). Equations (7) and (9) were derived from different approaches and converge to identical equations.

Originally, the effective viscosity term was brought to attention by Brinkman [9] when he mentioned the diffusion term to the original Darcy's law. However, the evaluation method of this effective viscosity was not established.

The use of effective viscosity for the diffusion term is of course more preferable. This viscosity is not necessary to be uniform for all directions as shown in Equation (9). Consequently, the effective viscosity might not be considered as a physical property of the fluid. Taking the form of the dispersion coefficient tensor given by Liu and Masliyah [2], effective viscosity can be evaluated. Using spherical particles in which their tortuosity is unique, and stating steady state condition of the flow, a present developed mathematical model of the momentum equation for the flow in porous media is formulated as the following

$$\frac{\partial}{\partial t}\rho\vartheta_i + \nabla\bullet\left(\frac{\rho\vartheta_i\vartheta_j}{\varepsilon}\right) = \nabla\bullet\mu_{eff}\left[\left(\nabla\vartheta_i\right) + \left(\nabla\vartheta_j\right)^T\right] - \nabla p - \rho g + \mu F\vartheta_i \qquad (10)$$

The momentum equations above can be further developed to the forms of specific models. The shear factor model is one of the forms to be introduced in momentum equation for covering the effect of fluid flow and solid interaction in porous media. Equation (10) above improves conventional models by including the convection term (which is usually excluded), and the diffusion term. At steady state condition and two-dimensional direction in axial and radial position, Equation (10) can be written in the full forms without gravitational force as the following:

- axial direction:

$$\frac{1}{\varepsilon}\frac{\partial}{\partial z}(\rho uu) + \frac{1}{\varepsilon}\frac{\partial}{\partial r}(\rho vu) = \frac{\partial}{\partial z}\left(\mu_{eff}\frac{\partial u}{\partial z}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\mu_{eff}\frac{\partial u}{\partial r}\right) - \frac{\partial p}{\partial z} + Fu \qquad (11)$$

- radial direction:

$$\frac{1}{\varepsilon}\frac{\partial}{\partial z}(\rho uv) + \frac{1}{\varepsilon}\frac{\partial}{\partial r}(\rho vv) = \frac{\partial}{\partial z}\left(\mu_{eff}\frac{\partial v}{\partial z}\right) + \frac{\partial}{\partial r}\left(\frac{\mu_{eff}}{r}\frac{\partial}{\partial r}(rv)\right) - \frac{\partial p}{\partial r} + Fv \qquad (12)$$

Equations (11) and (12) can be simplified in flux variables as follows:

$$J_{uz} = \frac{1}{\varepsilon}\rho uu - \left(\mu_{eff}\frac{\partial u}{\partial z}\right); \qquad J_{ur} = \frac{1}{\varepsilon}\rho vu - \left(\mu_{eff}\frac{\partial u}{\partial r}\right) \qquad (13)$$

$$J_{vz} = \frac{1}{\varepsilon}\rho uv - \left(\mu_{eff}\frac{\partial v}{\partial z}\right) \quad ; \quad J_{vr} = \frac{1}{\varepsilon}\rho vv - \left(\mu_{eff}\frac{\partial v}{\partial r}\right) \tag{14}$$

$$S_u = Fu \quad ; \quad S_v = Fv \tag{15}$$

Therefore, Equation (11) becomes

$$\frac{\partial}{\partial z}(J_{uz}) + \frac{1}{r}\frac{\partial}{\partial r}(rJ_{ur}) = -\frac{\partial P}{\partial z} + S_u \tag{16}$$

and Equation (12) becomes

$$\frac{\partial}{\partial z}(J_{vz}) + \frac{1}{r}\frac{\partial}{\partial r}(rJ_{vr}) = -\frac{\partial P}{\partial r} + S_v \tag{17}$$

Fu and *Fv* terms in momentum equations are mathematical models for momentum loss due to a fluid and solid interaction**s** in porous media. This term acts as a source term in the momentum equation. Factor *F* is called as a shear factor, Liu and Masliyah [2].

Shear factor or modified friction factor can be determined experimentally or theoretically. Shear factor is determined by the flow regime, porous media characteristics and fluid properties. Ideally, one would like to use heuristic arguments to derive an expression for shear factor in terms of universal constants and easily measurable properties of the porous material and the flowing fluid. Many investigators, like Ergun [10], Mc. Donald [11], Liu et al. [12] and Liu dan Masliyah [2], focused their research on the shear factor formulation itself. Various shear factor models are shown in Table 1. The performance of each shear factor for the solution of the momentum equations will be investigated here.

Table 1 Various shear factor models.

Shear Factor model	**Equation**	
Darcy	$F = -\frac{\mu}{k}$	(18)
Forchheimer	$F = \alpha + \beta u$	(19)
Brinkman (1947)	$F = -\frac{\mu}{k} + \mu\frac{\nabla^2 u}{u}$	(20)

Shear Factor model	Equation
Ergun (1952)	$$F = 150\frac{\mu(1-\varepsilon)^2}{d_p{}^2\varepsilon^3} + 1,75\frac{(1-\varepsilon)\rho u}{d_p\varepsilon^3} \quad (21)$$
Modified Ergun, Mc.Donald et al. (1979)	$$F = \left\{\frac{\mu}{R^2}\frac{(1-\varepsilon)^2}{\varepsilon^3 d_s{}^2}\right\} \left\{37,5\left[1+\frac{\pi d_s}{6(1-\varepsilon)}\right]^2 + 0,44\left[1-\frac{(1-0,5d_s)\pi^2 d_s}{24}\right]\left[\frac{\varepsilon^{1/6}\mathrm{Re}_m}{1+(1-\varepsilon^{1/2})^{1/2}}\right]\right\} \quad (22)$$
Liu, et al (1994)	$$F = \left(\frac{\mu(1-\varepsilon)^2}{4R^2 ds^2\varepsilon^{11/3}}\right) \left\{A\left(1+\frac{\pi d_s}{6(1-\varepsilon)}\right)^2 + 0.69\left(1-\frac{\pi^2 d_s}{24}(1-0.5d_s)\right)\mathrm{Re}_m\frac{\mathrm{Re}_m^2}{16^2+\mathrm{Re}_m^2}\right\} \quad (23)$$
Liu and Masliyah (1999)	$$F = \left(0,048\frac{1+0,46s_\Phi(1-\varepsilon^{1/2})^{1/2}}{s_\Phi}\left(\frac{(\mathrm{Re}-3)\,\mathrm{Re}^2}{36+\mathrm{Re}^2}\right) + 0,64 + \frac{0,363}{s_\Phi}\right)\left(\frac{18(1-\varepsilon)}{\varepsilon^{29/6}d_p^2}\right) \quad (24)$$

3 Numerical Method

The equations (4), (11) and (12) will be solved by numerical method in two-dimensional direction and cylindrical coordinate. Computation of conservation equations-above has been done by numerical Finite Volume Method [13]. In this method, the integral approach is done to discrete the conservation equations. First, calculate the domain, then discretize the domain in grid points. The region around the grid points is called control volume. The conservation laws must be valid in each control volume.

Momentum and continuity equations are arranged until they produce linear algebra equations. Those equations are solved with iterative method called line-by-line method. This method includes tridiagonal matrix that can be solved by Tridiagonal Matrix Algorithm (TDMA). The computation will be considered line-by-line following region of grid point. Initially, this computation is applied for sweeping from top to bottom and then from left to right. These two types of sweeping must be applied to *U*, *V* and *p* and are considered as one-iteration. Furthermore, this iteration will be continued until convergence.

Discretization for momentum equation will have additional term namely source term. Special method used to solve this equation is by accomplishing initial predictive pressure field. Subsequently, this discrete equation is solved to obtain initial value from velocity field value. The discretized pressure equation has been solved to obtain velocity correction equation and then actual pressure and velocity will be renewable. This algorithm has been called *Semi-Implicit Method for Pressure-Linked Equations* (SIMPLE), Patankar [13].

Source term is an influential term in those equations solution. The source term must be linearized to avoid unrealistic computation result. Source term is linearized, as Patankar [13]:

$$S = S_C + S_P \vartheta_P \tag{25}$$

The coefficient S_p value must be less or equal than zero. If S_p were positive, the physical situation could become unstable. From various linearization method, the result of the best realistic are obtained when the source term is linearized, with Patankar [13]:

$$S = S^* + \left(\frac{dS}{d\vartheta}\right)^* \left(\vartheta_P - \vartheta_P^*\right) \tag{26}$$

The symbol ϑ_P^* denotes the previous-iteration value of ϑ_P.

The convergence criteria are based on the residuals of the algebraic equations for solved variables. The algebraic equations are resulted from the discretization of one continuity equation for pressure correction and two momentum equations for u and v velocity components. The pressure correction at the centre of a control volume $p_P^{'}$ is an algebraic function of the pressure corrections of its control volumes $p_{nb}^{'}$. The pressure correction equation is written as

$$a_P p_P^{'} = a_E p_E^{'} + a_W p_W^{'} + a_N p_N^{'} + a_S p_S^{'} + b \tag{27}$$

where p'_{nb} are p'_e, p'_w, p'_n and p'_s. The term b in the pressure correction equation is the mass flow rate imbalance in the control volume of P. For a converged solution, the value of b should be zero theoretically and should be small enough numerically. A criterion for a convergence solution is set when the summation of b values for all control volumes are less than a small error value ε. This criterion is defined as follows

$$b_{sum} = \sum_{i_{cv}}^{N_{cv}} a_P p'_P - a_e p'_e + a_w p'_w + a_n p'_n + a_s p'_s {}_{i_{cv}} \qquad (28)$$

A small error value ε is set to 10^{-6}, then the solution converges if

$$b_{sum} < \varepsilon \qquad (29)$$

4 Non-uniform Porosity of Fixed Bed Media

For a fixed bed, there is a marked difference between the solid matrix structure near the containing wall and that in the bulk. This difference is better described by a porosity variation. For the first few particle thickness near the bounding wall, the volume-averaged porosity is higher than that in the bulk, which can render higher portion of the fluid to pass through this region. This behavior has been well characterized by Vortmeyer and Schuster [14]. When annular averaging is performed with a rather small band in the radial direction, one can also observe a fluctuation in the fluid flux near the wall region. This behavior is due to the porosity variation in the near wall region. The explanation of this behavior is well known: the layer of particles in contact with the wall is forced to be well ordered. The layer itself is less smooth than the wall and can only induce a weaker order on the adjacent layer. Hence, the degree of order decreases as the distance from the wall increases. While normally the spatial oscillation is considered to be removed when volume averaging is applied, there are cases where the spatial oscillation may be important. Therefore, it is necessary to treat the porosity variations in the near wall region.

Based on the exponential decay and co-sinusoidal concept, Liu and Masliyah [2] found a mathematical model that have a better fit to the experimental data for a packed beds of uniform spheres and cylinder as the following:

$$\varepsilon = \varepsilon_b + \frac{1-\varepsilon_b}{2} E_r \left[(1-0{,}3 p_d) \cos\left(\frac{2\pi}{1+1{,}6 Er^2} \frac{D/2-r}{p_d d_s} \right) + 0{,}3 p_d \right] \qquad (30)$$

$$E_r = \exp\left[-1,2\,p_d\left(\frac{D/2-r}{d_s}\right)^{3/4}\right] \quad (31)$$

Where D is the diameter of the column; ε_b is the porosity in the bulk region; p_d is the period of oscillation normalized by d_s, and E_r is an exponential decaying function that is defined by Equation (30). For a packed bed of uniform spheres, the period of oscillation is found to be 0,94 sphere diameter, Liu and Masliyah [2]. One can observe that Equation (30) characterizes the oscillation and decay quite well. For the next step, Equation (30) will be used in computation program.

5 Results and Discussions

The computational parameters were set to be the same as experimental parameters of Kufner and Hofmann [6]. Four shear factor models in Equations (21), (22), (23) and (24) were introduced in the momentum equation. The computation results of fluid flow field inside packed beds are compared to the experimental data of Kufner and Hofmann [6] and Stephenson and Stewart [7]. The experimental parameters of these data are given in Table 2.

Table 2 Parameters of the literature experimental data.

	Data from Kufner and Hofmann [6]	**Data from Stephenson and Stewart [7]**
Fluid	Air	Mixture of cyclooctane and cyclooctene
Fluid viscosity (μ)	1.7894 x 10^{-5} kg/m.s	2.42 x 10^{-3} kg/m.s
Fluid density (ρ)	1.225 kg/m^3	834.3 kg/m^3
Reactor diameter (D)	20 mm	75.7 mm
Particle diameter (d_p)	4.5 mm	7.035 mm
Reynolds number (Re)	2285	2549
D/d_p	4.44	10.7
Average feed velocity (U_{avg})	1.883 m/s	0.097 m/s
Bulk porosity (ε_b)	0.349	0.354

The results in Figure 1 show the axial flow velocity profiles of air flow through the packed bed of spheres. These profiles were computed for particle diameter d_p=4.5 mm, pipe diameter D=20 mm, average feed velocity (q) 1,883 m/s, and bulk porosity (ε_b) 0,4167. The Reynold number of this flow is 2285. Figure 3 shows the radial velocity component profile. These figures indicate that velocity profile produces the trend of having global maximum and minimum peaks at a distance very close to the wall. Generally, the numerical solution**s** of all of shear factor models agree with the experimental data.

In accordance with Kufner and Hofmann's data, the first maximum and minimum peak should occur at distance 0.22 d_p and 0.66 d_p from the wall. This value becomes a critical criterion in comparing the predicted results using various shear factor models and experimental results. This computation results give the first maximum peak at distance 0.17-0.22d_p and the first minimum peak at 0.60-0.62d_p. This means that in term of the quantity, these computational results are quite accurate.

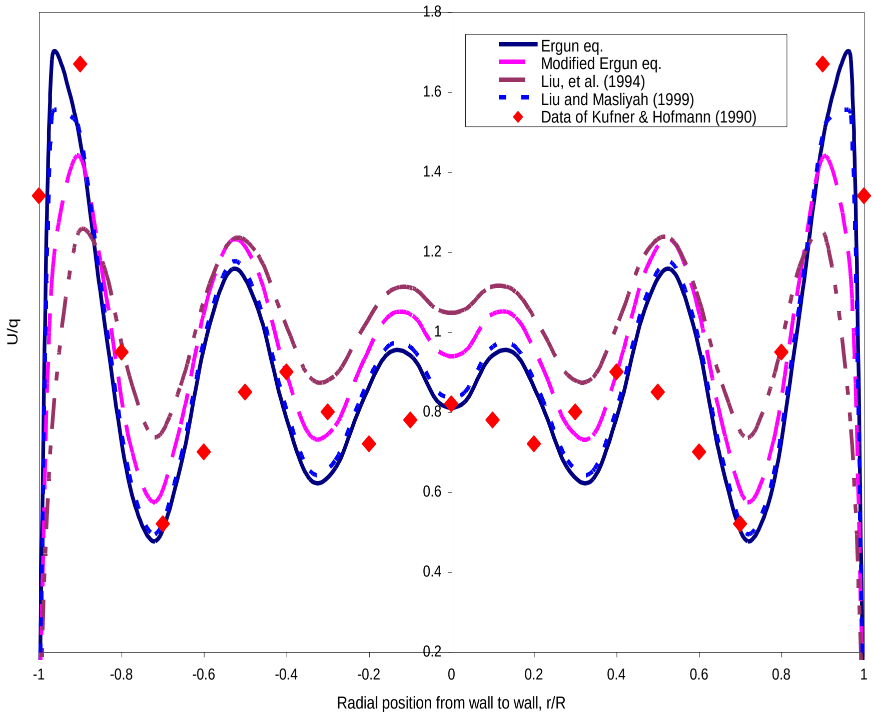

Figure 1 Axial flow velocity distribution for flow through a packed bed**.**

The comparison of present numerical modeling results with experimental data leads to some important findings. The convection and the diffusion terms in the mathematical modeling can be solved numerically and need not to be excluded. The effect of these terms to the flow field prediction exists especially to complex flow configuration that cannot be simplified in one-dimensional approach. Furthermore, the radial velocity profile can be predicted in which its importance is very clear for the real flow, and two or three-dimensional flow. There are various non-ideal problems of the flow in porous media that can be investigated using this numerical model.

Various shear factor formulas were investigated using this numerical solver. The performance of each shear factor was shown by Figure 1 and Figure 2 Compared to the the experimental data, the predicted axial velocity profiles for the same case as experimental case, Liu and Masliyah shear factor formula gives a better prediction for the velocity than other shear factors. One of the reasons is that Liu and Masliyah shear factor was developed as an improved shear factor from others.

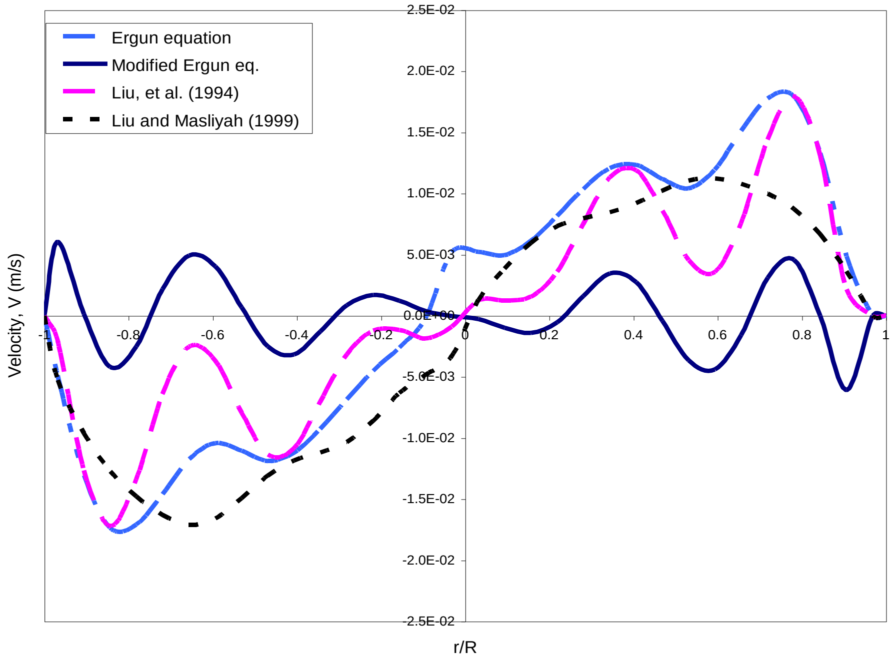

Figure 2 Radial flow velocity distribution for fluid flow through a packed bed.

Effect of effective viscosity of diffusion term on momentum equation has been investigated. Effective viscosity model, Equation (9), and Liu and Masliyah, Equation (24), shear factor were implemented in this computational work.

Figure 3 shows the comparison of the effect of the dynamic viscosity and the effective viscosity on axial velocity profile. Computation results show good agreement with experimental results of Kuffner and Hofmann [6] when the dynamic viscosity is used for prediction of peak velocity near the wall. When using an effective viscosity, Kuffner and Hofmann used a low tube to particle diameter ratio, which is 4.44. Hence the space distance between particles is considered to be wide. In such that condition the effect of the solid matrix resistance becomes smaller and leads to small addition to viscosity.

The influence of effective viscosity to axial velocity profile is more pronounced for the case of a high tube to particle diameter ratio, Figure 4. Experimental data of Stephenson and Stewart [7] are used for comparison. Figure 4 shows the comparison of influence of the dynamic viscosity and the effective viscosity on axial velocity profile for a mixture of cyclooctane and cyclooctene flows through the packed bed of spheres with d_p=7.0355 mm; D=75.7 mm, average feed velocity q=0.097 m/s, ε_b=0.354 and Re=2549. The D/d_p value of experimental data of Stephenson and Stewart is 10.7. Hence the space between particles is smaller than that of the experimental data of Kuffner and Hofmann.

The higher the D/d_p value, the smaller the space between particles in packed beds and the higher the resistance of the solid matrix. Therefore the influence of porous viscosity to the fluid flow field will be more significant. The presence of the solid matrix itself contributes to the significant addition to the viscosity on the diffusion term of flow as is called effective viscosity.

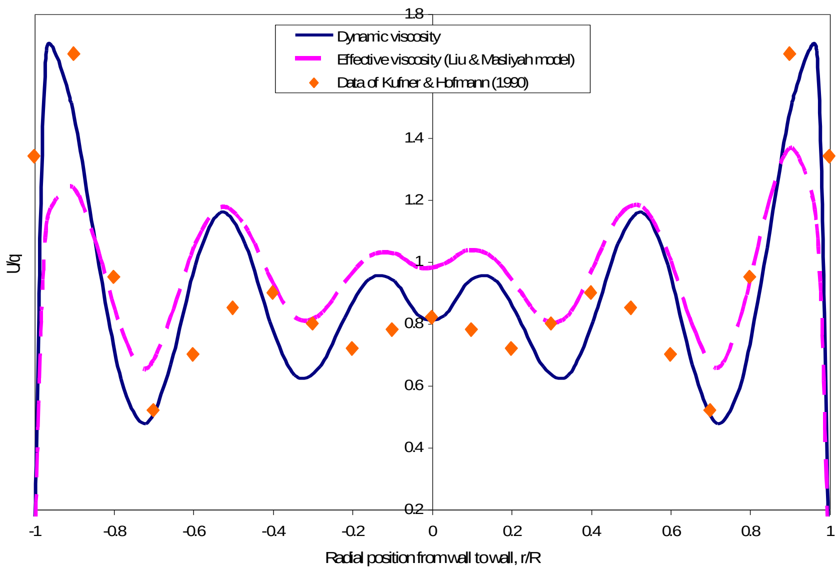

Figure 3 Influence of effective viscosity to axial velocity profile with low tube to particle diameter ratio (D/d_p=4.44).

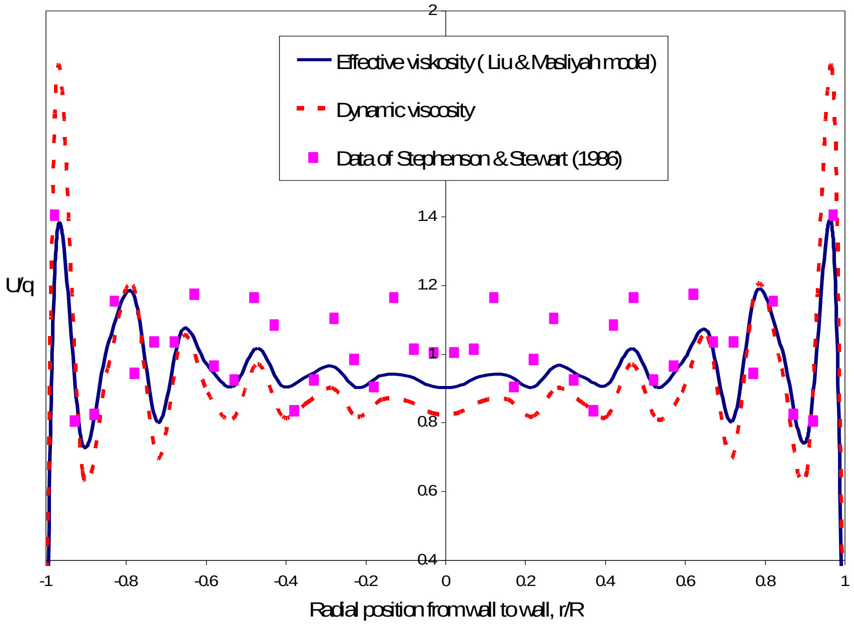

Figure 4 Influence of effective viscosity to axial velocity profile with high tube to particle diameter ratio (D/d_p=10.7).

6 Conclusions

A specific mathematical model for prediction of fluid flow field in porous media has been developed from a general and theoretical base momentum equation of fluid flow in porous media. The main principle of this mathematical flow model in the porous media is in additional term called a shear term which is a function its own velocity component and an effective viscosity involvement. A two dimensional numerical solution for this kind of flow has been constructed using finite volume method. The numerical results for the velocity distribution show a good agreement with the experimental data. The flow field profiles on axial direction agree well with the existing literature experimental data. It is observed that the first maximum peak occurs at distance of 0,17-0.22d_p; the second maximum peak occurs at distance of 1.00-1.02d_p and the first minimum peak occurs at distance of 0.60-0.62d_p. More comprehensive shear factor formulation results a better velocity production than other correlations do. The numerical study shows that the influence of effective viscosity to the velocity profile is more pronounced for higher diameter ratio of tube to particle.

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Notation

D = reactor diameter, m
d_p = particle diameter, m
d_s = D/d_p
F = shear factor
g = gravity force, m/s^2
L = packed length, m
p = pressure, $kg/m.s^2$
q = average feed velocity, m/s
r = radial position,m
R = reactor radius, m
Re = Reynolds number
U = superficial velocity x-direction, m/s
V = superficial velocity y-direction, m/s
ϑ_i = vector velocity
ε = porosity
μ = fluid viscosity, kg/m.s
ρ = fluid density, kg/m^3

References

1. Giese, M., Rottschafer, K. and Vortmeyer, D., *Measured and Modeled Superficial Flow Profiles in Packed Beds with Liquid Flow*, AIChE Journal, **44**(2), pp. 484-490, 1998.
2. Liu, S. & Masliyah, J.H., *Non-linear Flows in Porous Media*, Journal of Non-Newtonian Fluid Mechanics, **86**, pp. 229-252, 1999.
3. Stanek, V. & Szekely, J., *Three-dimensional Flow of Fluids through Non-uniform Packed Beds*, AIChE Journal, **20**(5), pp. 974-980, 1974.
4. Papageorgiu, J.N. and Froment, G.F., *Simulation Models Accounting for Radial Voidage Profiles in Fixed Bed Reactors*, Chem. Eng. Sci., **50**(19), pp. 3043-3056, 1995.
5. Benenati, R.F. and Brosilow, C.B., *Void Fraction Distribution in Beds of Spheres,* AIChE Journal, Vol. 8, No. 3, pp. 359-361, 1962.
6. Kufner, R. & Hofmann, H., *Implementation of Radial Porosity and Velocity Distribution in a Reactor Model for Heteregoneous Catalytic Gas Phase Reactions (Torus-Model)*, Chemical Engineering Science, **45**, pp. 2141-2146, 1990.
7. Stephenson, J.L. and Stewart, W.E, *Optical Measurements of Porosity and Fluid Motion in Packed Beds*, Chemical Engineering Science., **41**(8), 2161, 1986

8. Supardan, D., *Mathematical and Numerical Modeling of Fluid Flow in Porous Media Involving Shear Factor Models*, Master Thesis, Departement of Chemical Engineering, ITB, 2000.
9. Brinkman, H.C., *A Calculation of the Viscous Force Extended by a Flowing Fluid on a Dense Swarm of Particles*, Appl. Sci. Res., **A1**, pp. 27, 1947
10. Ergun, S, 1952, *Fluid Flow through Packed Columns*, Chem Eng. Prog., **48**, pp. 89, 1952
11. McDonald, I.F. , El-Sayed, M.S., Mow, K. & Dullien, F.A.L., *Flow through Porous Media-The Ergun Equation Revisited*, Ind. Eng. Chem. Fundamental, **18**, pp. 199-208, 1979.
12. Liu, S., Afacan, A. & Masliyah, J.H., 1, *Steady Incompressible Laminar Flow in Porous Media*, Chemical Engineering Science., **49**(21), pp. 3565-3586, 1994.
13. Patankar, S.V., 1, *Numerical Heat Transfer and Fluid Flow*, New York, Hemisphere Publishing Corporation, 1980.
14. Vortmeyer, D. & Schuster, J., *Evaluation of Steady Flow Profiles in Rectangular and Circular Packed Beds by a Variational Method*, Chemical Engineering Science, **38**, pp. 1691-1699, 1983.