

## PRECONDITIONED MULTIGRID METHOD FOR FLUID FLOW IN POROUS MEDIA

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### ABSTRACT

An efficient numerical approach is developed for modeling three-dimensional gas flow in porous media, based on the preconditioning method and a multigrid acceleration technique. An implicit approximate factorization (AF) method is used to solve the algebraic equation system and achieve computational efficiency. A new bound criterion is proposed for the selection of the pseudo-compressibility constant. The application of this approach is discussed with some illustrative examples.

Keywords: Preconditioning method, approximate factorization, multigrid, fluid flow, porous media

### NOMENCLATURE

CFL	Courant number
$d_p$	particle diameter
$P$	pressure
$S_i$ (I=1-6)	areas of computational cell
$t, \tau$	time
$u, v, w$	axial, circumferential and normal velocity components in the Navier-Stokes equation
$U, V, W$	contravariant velocities of the transformed Navier-Stokes equations
$x, y, z$	physical Cartesian coordinates
$\Omega$	cell volume
$\varepsilon$	porosity
$\phi$	particle sphericity
$\gamma$	kinematic viscosity
$\rho$	density
$\xi, \eta, \zeta$	transformed coordinates

### INTRODUCTION

Fluid flow in porous media is important in numerous industrial processes. While assumptions such as axial symmetry are often applied to reduce computational effort, in some processes like, for example, blast furnace, the fluid flow (and general operating) characteristics are best represented in three-dimensional coordinates. Two numerical methods have commonly been used to simulate fluid flow in such a process. One is based on the simplified stream function (Wang et al., 1997), and the other, on the Navier-Stokes equation (Zhang et al., 1998). For two-dimensional problems, the stream function approach is readily implemented; however, its application to three-dimensional problems is not straightforward. Conversely, the Navier-Stokes equation, using primitive variables (velocity and pressure), is commonly employed to describe a three-dimensional flow field. The flow equations are solved using a pressure-based solver and in general, a relaxation scheme is required iterating on pressure-correction until a zero-divergence condition is

reasonably realized. Computational effort required for simulating complex three-dimensional flows by this approach is quite significant and new solution methodologies are therefore highly desired.

Among the many methods developed to solve the incompressible Navier-Stokes equation, the pressure-based approach and artificial compressibility approach are perhaps the most successful. The pressure-based methods represented by the SIMPLE-family of codes were originated by Patankar et al. (1972). The preconditioned method, sometimes referred to as the artificial compressibility method and first proposed by Chorin (1967), has gained more acceptances recently, partly due to the success of the time-stepping scheme in simulating transient flows. In this method, an artificial time derivative of pressure is added to the continuity equation corrected with a pseudo-compressibility constant. The resulting system of equations is hyperbolic for the inviscid terms. Thus, the system is well posed and efficient numerical methods for compressible flows can be used to advance the system with an artificial time. Later, Turkel (1987) extended this concept and derived more sophisticated preconditions that render the new equation system well conditioned for numerical computation. To date, the method has been widely used to simulate single-phase flows with special reference to aerodynamics and hydrodynamics (Chang et al., 1984 and 1985; Rogers et al., 1985; Kwak et al., 1986; Sung et al., 1991; Zheng et al., 1997).

In this paper, a preconditioned multigrid numerical technique is described and applied to the simulation of fluid flow in porous media. The mathematical formulation and numerical methods employed are first described. Their application is then demonstrated via computations of gas flows in two-dimensional and three-dimensional packed beds, the latter under simplified blast furnace conditions.

### THEORETICAL TREATMENTS

#### Governing Equations

Based on the space-averaged theorem, a system of governing equations coupled with the drag force estimated by the Egrun equation in cartesian coordinates for fluid flow in porous media, can be written as (Fletcher, 1991):

$$\frac{\partial E}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} + \frac{\partial H}{\partial z} = \frac{\partial F_v}{\partial x} + \frac{\partial G_v}{\partial y} + \frac{\partial H_v}{\partial z} + D_i \quad (1)$$

where

$$D_f = -fE, f = \frac{150(1-\varepsilon)^2 v}{\varepsilon(\phi_p d_p)^2} + \frac{1.75(1-\varepsilon)\sqrt{u^2 + v^2 + w^2}}{\varepsilon\phi_p d_p} \quad (2)$$

$$E = [0 \quad u \quad v \quad w]^T \quad (3)$$

$$F = \begin{bmatrix} u \\ u^2 + p \\ uv \\ uw \end{bmatrix}, G = \begin{bmatrix} v \\ vu \\ v^2 + p \\ vw \end{bmatrix}, H = \begin{bmatrix} w \\ wu \\ wv \\ w^2 + p \end{bmatrix} \quad (4)$$

$$F_v = v \begin{bmatrix} 0 \\ 2u_x \\ u_y + v_x \\ u_z + w_x \end{bmatrix}, G_v = v \begin{bmatrix} 0 \\ v_x + u_y \\ 2v_y \\ v_z + w_y \end{bmatrix}, H_v = v \begin{bmatrix} 0 \\ w_x + u_z \\ w_y + v_z \\ 2w_z \end{bmatrix} \quad (5)$$

where  $D_f$  is the drag force;  $E$  the dependent variable;  $F$ ,  $G$  and  $H$  the convective fluxes; and  $F_v$ ,  $G_v$  and  $H_v$  are diffusive fluxes. Note that  $p$  represents  $P\varepsilon/\rho$ .

### Preconditioning Method

The above modified Navier-Stokes equations can be solved using the preconditioning method. This approach was originally used to obtain steady-state solutions of the incompressible Navier-Stokes equations by directly coupling the pressure and velocity fields. As shown below, it can be extended to simulate the fluid flow in a porous medium.

According to this approach, the continuity equation in Cartesian coordinates is

$$p_i = -\beta(u_x + v_y + w_z), \quad \beta \gg 1 \quad (6)$$

where  $\beta$  is the pseudo-compressibility parameter. In order to accommodate generalized three-dimensional curvilinear coordinates, the following independent variables are introduced:

$$\begin{cases} \tau = t \\ \xi = \xi(x, y, z, t) \\ \eta = \eta(x, y, z, t) \\ \zeta = \zeta(x, y, z, t) \end{cases} \quad (7)$$

The so-called Chorin-type preconditioning method is employed in this work. Thus, Eq. (1), i.e. the modified incompressible Navier-Stokes equations, with the pseudo-compressibility term included, can be rewritten as

$$\frac{\partial \hat{D}}{\partial \tau} + \frac{\partial}{\partial \xi}(\hat{F} - \hat{F}_v) + \frac{\partial}{\partial \eta}(\hat{G} - \hat{G}_v) + \frac{\partial}{\partial \zeta}(\hat{H} - \hat{H}_v) = D_f \quad (8)$$

where

$$\hat{D} = \frac{1}{J} [p \quad u \quad v \quad w]^T, \quad D = J\hat{D} \quad (9)$$

$$\hat{F} = \frac{1}{J} \begin{bmatrix} \beta U + \xi_i(p - \beta) \\ uU + \xi_x p \\ vU + \xi_y p \\ wU + \xi_z p \end{bmatrix} \quad (10a)$$

$$\hat{G} = \frac{1}{J} \begin{bmatrix} \beta V + \eta_i(p - \beta) \\ uV + \eta_x p \\ vV + \eta_y p \\ wV + \eta_z p \end{bmatrix} \quad (10b)$$

$$\hat{H} = \frac{1}{J} \begin{bmatrix} \beta W + \zeta_i(p - \beta) \\ uW + \zeta_x p \\ vW + \zeta_y p \\ wW + \zeta_z p \end{bmatrix} \quad (10c)$$

and where the transformation Jacobian is defined as

$$J = \det \frac{\partial(\xi, \eta, \zeta)}{\partial(x, y, z)} = \begin{vmatrix} \xi_x & \xi_y & \xi_z \\ \eta_x & \eta_y & \eta_z \\ \zeta_x & \zeta_y & \zeta_z \end{vmatrix} \quad (11)$$

and

$$\begin{cases} U = \xi_t + \xi_x u + \xi_y v + \xi_z w \\ V = \eta_t + \eta_x u + \eta_y v + \eta_z w \\ W = \zeta_t + \zeta_x u + \zeta_y v + \zeta_z w \end{cases} \quad (12)$$

In this case, the viscous terms are given by

$$\begin{aligned} \hat{F}_v &= \frac{v}{J} (\nabla \xi \cdot \nabla \xi I_m \frac{\partial D}{\partial \xi} + \nabla \xi \cdot \nabla \eta I_m \frac{\partial D}{\partial \eta} + \nabla \xi \cdot \nabla \zeta I_m \frac{\partial D}{\partial \zeta}) \\ \hat{G}_v &= \frac{v}{J} (\nabla \eta \cdot \nabla \xi I_m \frac{\partial D}{\partial \xi} + \nabla \eta \cdot \nabla \eta I_m \frac{\partial D}{\partial \eta} + \nabla \eta \cdot \nabla \zeta I_m \frac{\partial D}{\partial \zeta}) \\ \hat{H}_v &= \frac{v}{J} (\nabla \zeta \cdot \nabla \xi I_m \frac{\partial D}{\partial \xi} + \nabla \zeta \cdot \nabla \eta I_m \frac{\partial D}{\partial \eta} + \nabla \zeta \cdot \nabla \zeta I_m \frac{\partial D}{\partial \zeta}) \end{aligned} \quad (13)$$

where

$$I_m = \begin{vmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{vmatrix} \quad (14)$$

### Numerical Algorithm

The above equations are approximately factorized using the method of Beam and Warming (1976) and advanced in time using the following equation in delta form:

$$L_\xi L_\eta L_\zeta (D^{n+1} - D^n) = \text{RHS}^n \quad (15)$$

where  $D^n$  is the value of  $D$  at time  $\tau = n\Delta\tau$ , and

$$\begin{aligned} L_\xi &= I + \frac{\Delta\tau}{2} J \delta_\xi (\hat{L}_1 - \hat{F}_1) - \Delta\tau D_f I_m \\ L_\eta &= I + \frac{\Delta\tau}{2} J \delta_\eta (\hat{L}_2 - \hat{F}_2) - \Delta\tau D_f I_m \\ L_\zeta &= I + \frac{\Delta\tau}{2} J \delta_\zeta (\hat{L}_3 - \hat{F}_3) - \Delta\tau D_f I_m \end{aligned} \quad (16)$$

$$\begin{aligned} \text{RHS}^n &= -\Delta\tau J [\delta_\xi (\hat{F} - \hat{F}_v)^n + \delta_\eta (\hat{G} - \hat{G}_v) + \delta_\zeta (\hat{H} - \hat{H}_v)] \\ &\quad - \varepsilon_e [(\nabla_\xi \Delta_\xi)^2 + (\nabla_\eta \Delta_\eta)^2 + (\nabla_\zeta \Delta_\zeta)^2] C^n + \Delta\tau D_f I_m \end{aligned} \quad (17)$$

Here,  $\nabla$ ,  $\Delta$  and  $\delta$  are the backward-difference, forward-difference and central-difference operators, respectively, and  $I$  is the  $4 \times 4$  identity matrix. The Jacobian matrices are given by

$$\begin{aligned} \hat{L}_1 &= \frac{1}{J} \begin{vmatrix} \xi_x & \xi_x \beta & \xi_y \beta & \xi_z \beta \\ \xi_x & U + \xi_x u & \xi_y u & \xi_z u \\ \xi_y & \xi_x v & U + \xi_y v & \xi_z v \\ \xi_z & \xi_x w & \xi_y w & U + \xi_z w \end{vmatrix} \\ \hat{L}_2 &= \frac{1}{J} \begin{vmatrix} \xi_x & \eta_x \beta & \eta_y \beta & \eta_z \beta \\ \eta_x & V + \eta_x u & \eta_y u & \eta_z u \\ \eta_y & \eta_x v & V + \xi_y v & \eta_z v \\ \eta_z & \eta_x w & \eta_y w & V + \eta_z w \end{vmatrix} \\ \hat{L}_3 &= \frac{1}{J} \begin{vmatrix} \zeta_x & \zeta_x \beta & \zeta_y \beta & \zeta_z \beta \\ \zeta_x & W + \zeta_x u & \zeta_y u & \zeta_z u \\ \zeta_y & \zeta_x v & W + \zeta_y v & \zeta_z v \\ \zeta_z & \zeta_x w & \zeta_y w & W + \zeta_z w \end{vmatrix} \end{aligned} \quad (18)$$

The viscous terms are

$$\begin{aligned}\hat{\Gamma}_1 &= \frac{\nu}{J} \nabla \xi \cdot \nabla \xi I_m \delta_\xi \\ \hat{\Gamma}_2 &= \frac{\nu}{J} \nabla \eta \cdot \nabla \eta I_m \delta_\eta \\ \hat{\Gamma}_3 &= \frac{\nu}{J} \nabla \zeta \cdot \nabla \zeta I_m \delta_\zeta\end{aligned}\quad (19)$$

and

$$C = [p \ 0 \ 0 \ 0]^T \quad (20)$$

which is a  $4 \times 4$  block tridiagonal system of equations. The approximate factorization (Eq. (15)), is implemented with a three-stage algorithm. The three stages are expressed as follows:

$$\begin{aligned}\left[ I + \frac{\Delta\tau}{2} J \delta_\xi (\hat{L}_1 - \hat{\Gamma}_1) - \Delta\tau D_r I_m \right] \overline{\overline{\Delta D}} &= \text{RHS}^n \\ \left[ I + \frac{\Delta\tau}{2} J \delta_\eta (\hat{L}_2 - \hat{\Gamma}_2) - \Delta\tau D_r I_m \right] \overline{\overline{\Delta D}} &= \overline{\overline{\Delta D}} \\ \left[ I + \frac{\Delta\tau}{2} J \delta_\zeta (\hat{L}_3 - \hat{\Gamma}_3) - \Delta\tau D_r I_m \right] \Delta D &= \overline{\overline{\Delta D}}\end{aligned}\quad (21)$$

In incompressible flows, there is usually no discontinuity phenomenon to consider, such as shock waves. High-resolution schemes, such as TVD (total variation diminishing) or eigenvalue-based upwind, are not necessary, because these schemes are quite expensive and are significant only near the shock wave. Therefore, for the fluid flow equations in porous media, a regular second-order central-difference differencing scheme is used. In this case, numerical dissipation terms are introduced to dampen out the high-frequency oscillation. The numerical dissipation or “smoothing” takes the form of a derivative of the variables in  $D$ . The artificial dissipation is designed for compressible flows. The second difference term is used to suppress overshooting caused by shocks and the fourth difference term is used to damp the spurious oscillations in the smooth region. Therefore, in this work the second difference term is neglected and the only fourth-order artificial dissipation terms are added to the system, as shown in Eq. (17). These terms only provide additional dissipation to suppress spurious numerical oscillations when the grid size is not small enough to render the physical viscosity effective. Therefore they will not contaminate the physical solutions, i.e. the resulting error due to this treatment can be reasonably ignored. The present numerical solutions also show the forth-order artificial dissipation terms do not affect the accuracy.

### Lower Bound of $\beta$

The basic knowledge for a successful application of the pseudo-compressibility to solving single-phase flow problems was presented by Chang et al., (1984). The criteria for properly selecting the pseudo-compressibility constant  $\beta$  were also investigated in detail (Chang et al., 1985; Kwak et al., 1986). When the method is extended to simulation of the fluid flow in a porous medium, a new range for  $\beta$  is necessary to avoid the stiffness of the algebraic equation system. In porous media, the behavior of fluid flow is significantly affected by the interaction force between particles and fluid. This force is implicitly treated in the discretization scheme with the AF method,

making the pseudo-compressible formulation very stiff as implied in Eq. (21). To overcome this, the pseudo-compressibility constant  $\beta$  should satisfy the following criterion:

$$\beta > f + 1 \quad (22)$$

where  $f$  is as defined in Eq. (2).

### Multigrid Techniques

The multigrid technique developed by Jameson (1985) is employed to speed up convergence. By the cyclic use of a sequence of fine to coarse grids, the technique is very effective in damping the solution modes with long wave lengths which are primarily responsible for slow convergence. In principle, the relation between fine and coarse grids is arbitrary. However, for ease of coding, a coarse grid is constructed from a fine grid by skipping every other grid point. Thus, the total number of cells in a coarse grid system is only half of the total number of the cells in the fine grid system. The time stepping is first performed on the finest grid. The solution is then transferred to the coarse grid. This process is repeated until the coarsest grid is reached. In the reverse process, from the coarsest grid to the finest grid, the corrections from a coarse grid are interpolated and then added to the old next finer grid variables to form a new finer grid solution. This process is again repeated until the finest grid is reached. No time stepping is performed in this process. However, the interpolated corrections are smoothed before they are added to the fine grid solution in order to reduce the errors caused by linear interpolation. Only V-cycle has been tested. The comparison of the rates of convergence of single grid and 3-level V-cycle multigrid has been performed in this work. The V-cycle multigrid is 2-3 times faster in CPU time than the single grid. In addition, local time stepping is also used to accelerate the rate of convergence. The local time step size is given by

$$\Delta\tau = \frac{\text{CFL} \cdot \Omega}{\max(u_c, v_c, w_c) \bar{S}} \quad (23)$$

where

$$\begin{aligned}u_c &= |u| + \sqrt{u^2 + \beta(\xi_x^2 + \xi_y^2 + \xi_z^2)} \\ v_c &= |v| + \sqrt{v^2 + \beta(\eta_x^2 + \eta_y^2 + \eta_z^2)}\end{aligned}\quad (24)$$

$$\begin{aligned}w_c &= |w| + \sqrt{w^2 + \beta(\zeta_x^2 + \zeta_y^2 + \zeta_z^2)} \\ \bar{S} &= \sum_{i=1}^6 S_i\end{aligned}\quad (25)$$

Notably, with the use of a dual-time stepping scheme and with some necessary modifications, the preconditioned approach can also deal with unsteady-state flow problems. In this case, a pseudo-time term is introduced to the above conservation of equation to fulfil a pseudo-time marching during each physical time step.

### Boundary Conditions

The boundary types encountered in this work are classified as solid wall, periodic, singularity and outlet. For viscous flow, a non-slip condition is imposed on the solid wall boundary by setting the flow velocity equal to that of the body, together with a zero pressure gradient normal to the

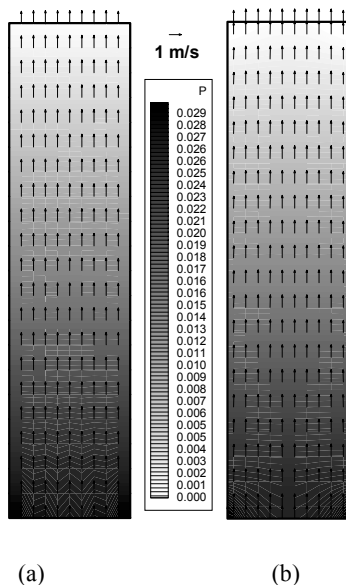
surface to determine the pressure on the wall. For inviscid flow, the normal velocity component is set to zero, the only contribution to the conservation law for a cell adjacent to the wall is the pressure on the wall, which can be obtained from the normal momentum equation.

Since a ghost cell is introduced to store the value and derivatives across the boundary, the boundary conditions for the symmetrical plane and periodical face can be readily accomplished by assigning the ghost cell with the value of its corresponding cell. Because there is no flux across singular, the boundary conditions for the singularity are obtained by extrapolation combined with partial averaging. At the outlet, the back pressure is given, and a fully developed flow condition is assumed.

## COMPUTATIONAL RESULTS

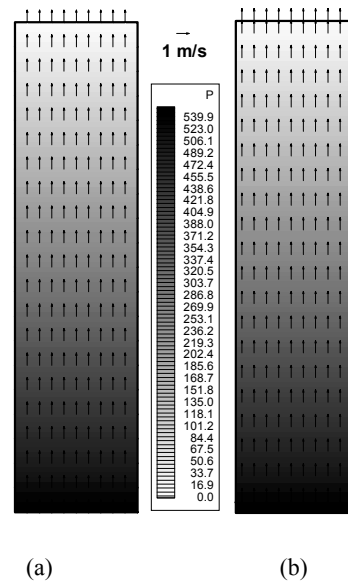
### Validation of the Proposed Approach

To test the flow solver, the gas flow through a two-dimensional rectangular packed bed is computed. The test case is a bed packed with particles of 0.003 m diameter. The bed is 0.4 m high and 0.1 m wide. Gas is introduced uniformly at the bottom, with velocity equal to 1 m/s. Figs. 1 (a) and 1 (b) show the pressure contours and velocity vectors in an empty bed, respectively, obtained using (a) the pseudo-compressibility approach, with  $\beta$  equal to 5, according to Rogers et al. (1985), and (b) the SIMPLE method, in which the overall velocity magnitude difference is less than  $10^{-9}$ .



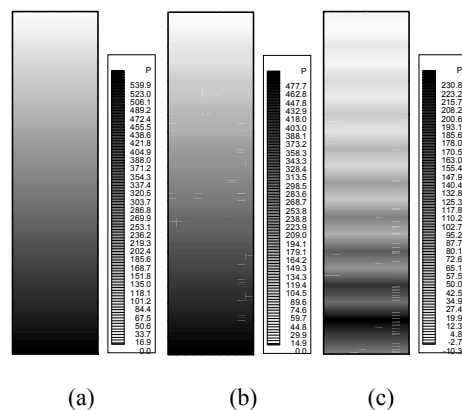
**Figure 1:** Pressure contours and velocity vectors in an empty bed, simulated by: (a), the pseudo-compressibility approach; (b), the SIMPLE method.

Similarly, Figs. 2 (a) and 2 (b), show the pressure contours and velocity vectors in the packed bed, respectively, again by the pseudo-compressibility approach where  $\beta$  is estimated as 500 according to Eq. (22) and the SIMPLE method, in which the overall velocity magnitude difference is less than  $10^{-7}$ . Obviously, there is a good agreement between the results computed by the two numerical methods. Since the applicability of the SIMPLE method has been well established, the agreement confirms the validity of the proposed approach.



**Figure 2:** Pressure contours and velocity vectors in a packed bed, simulated by: (a), the pseudo-compressibility approach; (b), the SIMPLE method.

The influence of  $\beta$  on the numerical accuracy is demonstrated in Fig. 3, which shows the calculated pressure field for different values of  $\beta$ . The results show that if  $\beta$  is too small, the solution does not converge, leading to an unrealistic pressure (and flow) field. They also confirm that in order to solve the stiff problem associated with the algebraic equation system,  $\beta$  must be greater than a threshold value, as given by Eq. (22).

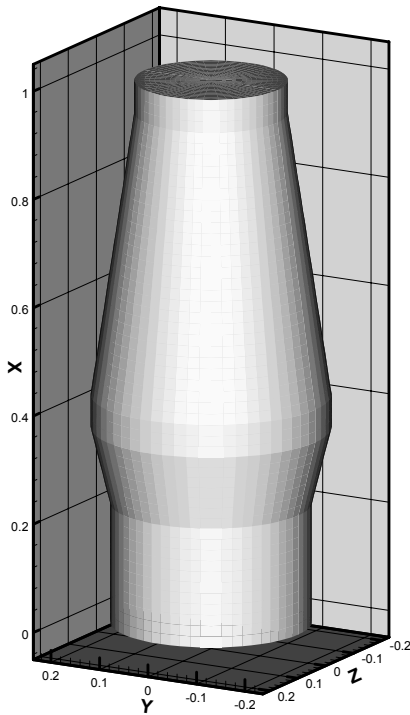


**Figure 3:** Pressure contours with three values of  $\beta$ : (a), 500; (b), 5; (c), 0.5.

### Application to Three-dimensional Gas Flow

The preconditioned, multigrid technique described above is now applied to the simulation of three-dimensional fluid flow in porous media, specifically, the three-dimensional flow of gas in an idealized blast furnace geometry (see Fig. 4). For simplicity, it is assumed that the blast furnace has six tuyeres or gas inlets which are uniformly located at  $x = 0.16$  m. Fig. 5 shows the velocity vectors at three different Y-Z planes in the blast furnace. Fig. 6 shows the pressure contours on the surface (wall) and the velocity vectors at a specified cross section in the blast furnace. These computed results are in general agreement with the observed data (Omori, 1987). Notably, unlike in an empty

blast furnace, the gas flow in the blast furnace demonstrates less re-circulating behavior near to the air inlets because the existence of packed particles enhances diffusion and weakens convection.

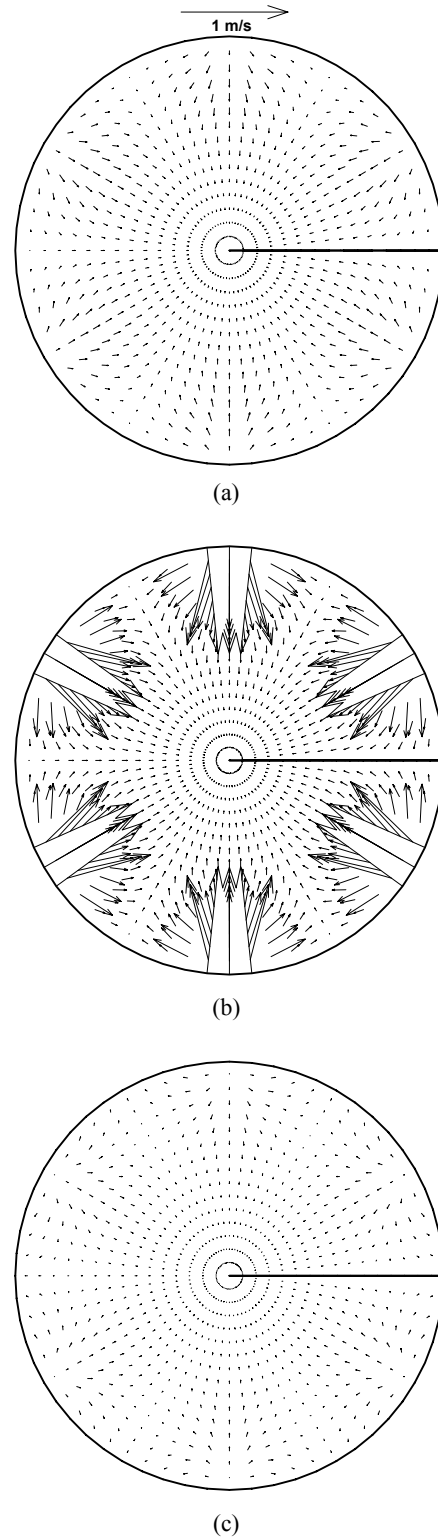


**Figure 4:** Three-dimensional blast furnace (m)

It has been widely recognized that the multigrid method can significantly accelerate the convergence rate of numerical solutions for the governing equations of fluid flow (Anderson et al., 1988; Jameson et al., 1984; Jameson et al., 1985; Ni, 1982). Furthermore, the implicit approximation factorization method (AF) which was originally developed to substitute for SLOR, ADI, SIP etc. to avoid the pressure-based approach has been proved to be highly efficient for the solution of fluid flow. The proposed approach is largely a direct application of the preconditioned multigrid method facilitated with the AF technique to fluid flow in porous media. Naturally, it should lead to a considerable reduction in computational effort. The present preliminary computation confirms this and a more detailed analysis will be available in the near future.

## CONCLUSIONS

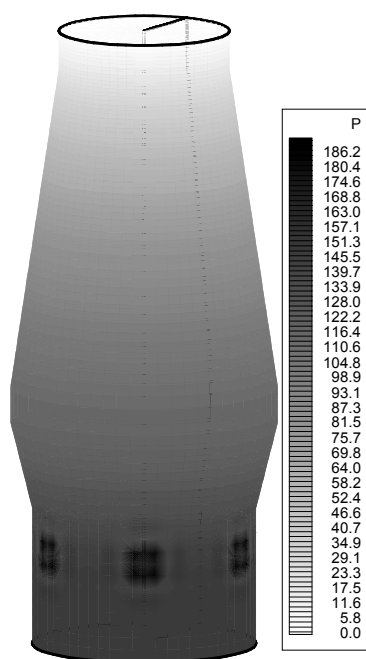
An efficient numerical approach based on the multigrid and preconditioning methods is proposed for predicting three-dimensional steady flows in porous media. It is found that the pseudo-compressibility constant is crucial to the success of the proposed approach. The criterion for selecting this constant is presented and verified. The test cases carried out so far demonstrate the accuracy and efficiency of the proposed approach, with the computed results comparable with those established either experimentally or computationally in the literature. The code should be useful for the three-dimensional simulation of fluid flow in packed bed reactors where high efficient computation is required.



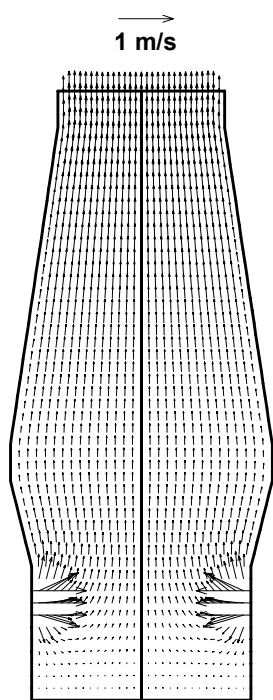
**Figure 5:** Velocity vectors in the blast furnace at three different planes: (a),  $x = 0.1$  m; (b),  $x = 0.16$  m; (c),  $x = 0.22$  m

## ACKNOWLEDGEMENTS

The authors would like to thank Australian Research Council and BHP for financial support.



(a)



(b)

**Figure 6:** (a), pressure contours on the surface and (b), velocity vectors on the plane across an inlet center and symmetrical axis

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