Efficient Modeling of Time-Dependent, Maldistributed Flow in Packed Beds

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INTRODUCTION

Fluid flow through packed beds with a spatially nonuniform resistance to flow is significant in many chemical reaction systems. In some applications this spatially nonuniform resistance is inherent in layer charged burdens, as in blast furnace operation. In other settings uniform packing is the ideal that cannot be realized, as in oil shale retorts. Where feasible, packed beds are often carefully filled to create or avoid these nonuniformities.

The mathematical description of packed-bed flow has been a subject of interest for many years. One of the most commonly used models to describe flow maldistributions is the vectorial, differential form of the Ergun equation:

$$-\nabla P = V(f_1 + f_2 V) \tag{1}$$

which evolved in a series of papers by Stanek and Szekely (1972, 1973, 1974). Shortly thereafter Szekely and Poveromo (1975) experimentally verified this approach and adapted Eq. 1 to model more closely the observed phenomena. These modifications were to describe better the wall effect (preferential flow near the wall due to a higher local void fraction) and the larger resistance to flow at the interface of regions composed of particles of different diameters.

The adaptation of Eq. 1 provides a foundation for describing chemical and thermal processes in packed beds. This approach has been used as the basis of several models describing many different processes. Various authors have considered the limitations of Eq. 1 and have studied the necessity and validity of extensions to more general problems. These include Choudary et al. (1976), who considered the inclusion of the inertial terms $\rho(V \cdot \nabla)V$ in Eq. 1, and Chandrasekhara and Vortmeyer (1979) who studied the addition of the viscous terms $\mu\nabla^2 V$. An extension of Eq. 1 to time-dependent problems in which body forces may be significant is proposed. Then an efficient scheme for the numerical solution of the equations is given.

FORMULATION

Consider the three-dimensional flow of fluid through a packed bed where the flow may be maldistributed. This flow maldistribution may be due to spatially variable porosity or particle size distribution, temperature gradients or the nonuniform introduction of the inlet gas. Equation 1 has been used to model this flow successfully in the steady state problem.

In large packed beds such as oil shale retorts, Eq. 1 must be generalized. Vertical in situ retorts may be deeper than 1,000 ft (305 m) and horizontal in situ retorts could be considerably longer. The major controlling devices for the chemical reactions in the retort are variable inlet gas velocity and composition. Materials produced and consumed may dynamically change the flow resistance. Even more difficult to deal with, the processes will not in general be even quasisteady, so an accurate model must be time-dependent and allow for gravitational effects. Thus the following model

$$\rho \frac{\partial V}{\partial t} = -\nabla P - V(f_1 + f_2 V) + \rho g \tag{2}$$

is used along with the continuity equation for an incompressible fluid:

$$\nabla \cdot V = 0 \tag{3}$$

Stanek and Szekely (1974) showed that for various values of the modified Reynolds number, simplifying assumptions could be made. In particular for $Re_m > 150$, the viscous dissipation is negligible. For this reason they omitted the viscous term f_1 in their computations. However in many oil shale retorting applications $Re_m < 150$, so both viscous and inertial dissipation terms will be significant. Thus both f_1 and f_2 are included in the computations.

TWO-DIMENSIONAL PROBLEM

Consider the two-dimensional problem in rectangular coordinates with $0 \le x \le W$, $0 \le y \le H$. To solve Eqs. 2 and 3, the following boundary conditions are used. For the velocities, no-slip walls are specified as

$$V = 0 \qquad \text{at } x = 0, x = W \tag{4a,b}$$

A time-dependent inlet flow is given as

$$V_y = V_y(t) \quad \text{and} \quad V_x = V_x(t) \qquad \text{at } y = 0 \tag{5a,b}$$

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with outlet conditions specifying parallel flow as

$$\frac{\partial V_y}{\partial y} = 0 \quad \text{and} \quad V_x = 0 \qquad \text{at } y = H \tag{6a,b}$$

Neumann boundary conditions for the pressure at the walls are

$$\frac{\partial P}{\partial x} = 0 \qquad \text{at } x = 0, x = W \tag{7a,b}$$

A reference pressure is specified at outlet as

$$P = 0 \qquad \text{at } y = H \tag{8}$$

while from Eq. 2 the inlet pressure gradient is

$$\frac{\partial P}{\partial y} = \rho g - V_y(f_1 + f_2 V) \qquad \text{at } y = 0 \tag{9}$$

For initial conditions a pressure gradient is imposed, and the corresponding steady state velocity profile is used. As in Szekely and Poveromo (1975), spatial nonuniformities in the resistance to flow were accounted for by position dependence of the resistance parameters f_1 and f_2.

NUMERICAL METHOD

The numerical solution of Eqs. 2 to 9 uses a different approach than previously considered. The scheme is extremely efficient and uses the unique character of Eq. 2. This decreases the computational labor for the time-dependent problem.

Equations 2 and 3 with the boundary conditions in Eqs. 4 to 9 were solved using a fractional step finite-difference scheme developed by Chorin (1967, 1968) for the time-dependent Navier-Stokes equations for an incompressible fluid. The method begins by writing an implicit scheme for Eqs. 2 and 3 as

$$\rho(V^{n+1} - V^n) = -\Delta t G P^{n+1} - \Delta t\, V^{n+1}(f_1 + f_2 V^{n+1}) + \Delta t \rho g \tag{10a}$$

and

$$D V^{n+1} = 0 \tag{10b}$$

where G and D are difference operators for the gradient and divergence, respectively. Equations 10a and 10b are then solved by first solving

$$\rho(V^{aux} - V^n) = \Delta t\, K(V^{aux}) \tag{11}$$

where

$$K(V) = -V(f_1 + f_2 V) + \rho g \tag{12}$$

Then $K(V^{aux})$ is decomposed into the sum of $\rho T V^{n+1}$ and GP^{n+1}, where T is a difference operator for the time derivative $\partial/\partial t$. If T is the backward difference operator, then from Eq. 11 this decomposition is equivalent to decomposing V^{aux} into V^{n+1} and $\Delta t/\rho G P^{n+1}$, which can be accomplished by the following iterations:

$$P^{n+1,1} = P^n \tag{13a}$$

$$P^{n+1,m+1} = P^{n+1,m} - \lambda D\, V^{n+1,m+1}, \quad m > 1 \tag{13b}$$

and

$$V^{n+1,m+1} = V^{aux} - \frac{\Delta t}{\rho} G^m P^{n+1}, \quad m > 1 \tag{13c}$$

where $G^m P^{n+1}$, which is a functon of $P^{n+1,m+1}$ and $P^{n+1,m}$, converges to GP^{n+1} as $|P^{n+1,m+1} - P^{n+1,m}|$ tends to zero. Clearly, Eqs. 13b and 13c illustrate that as the iteration in Eq. 13b converges, the continuity equation is satisfied and the decomposition is accomplished. Eqs. 11 and 13 approximate the solution of Eq. 10a to second order in time.

The special nature of Eq. 11 makes this method extremely efficient. Note that solving Eq. 11 can be algebraically reduced to the problem of solving a quadratic equation. Hence no numerical scheme is necessary. Equations 13 were solved directly, where for $G^m P^{n+1}$ second-order central differences were used with P^{n+1} at (i,j) represented by $\frac{1}{2}(P_{ij}^{n+1,m+1} + P_{ij}^{n+1,m})$ to speed convergence. At all other grid points, $P^{n+1,m}$ was used. It should be noted that $V^{n+1,m+1}$ need not be calculated at each iteration. Only after $P^{n+1,m+1}$ has converged is V^{n+1} calculated from Eq. 13c.

Another approach may also be used. When Eq. 13c is substituted into Eq. 13b, we obtain

$$P^{n+1,m+1} = P^{n+1,m} - \lambda D\, V^{aux} + \frac{\Delta t}{\rho} D G^m P^{n+1} \tag{14}$$

which is an iterative procedure for solving

$$L P^{n+1} = \frac{\rho}{\Delta t} D\, V^{aux} \tag{15}$$

where L is a difference operator for the Laplacian $L = DG$. Equation 15 is a finite-difference approximation to

$$\nabla^2 P^{n+1} = \frac{\rho}{\Delta t} \nabla \cdot V^{aux} \tag{16}$$

which can be obtained by taking the divergence of the decomposition

$$\rho \frac{\partial V^{aux}}{\partial t} = \rho \frac{\partial V^{n+1}}{\partial t} + \nabla P^{n+1} \tag{17}$$

Thus Eqs. 13 were also cast as the Poisson equation (16) and solved directly via an LU decomposition. It is seen that at each successive time step the original LU decomposition can be used, which significantly reduces computational labor. This second method of solving Eqs. 13 was found to be more efficient, and the computed results shown were calculated by this method.

This efficient numerical scheme has the flexibility of time-dependent inlet conditions when necessary, yet it limits the computational work for the steady state process that evolves. An 11 × 11 finite-difference grid was used, and second-order central differences for the spatial derivatives were employed. Boundary conditions were approximated to maintain the second-order accuracy.

COMPUTED RESULTS

Figure 1a illustrates the velocity redistribution that occurs at the inlet as a preferential flow in the region of less resistance is established. Further down the bed the flow is essentially parallel with some flow in the direction of the regions of less resistance. Clearly illustrated is the slower flow that occurs in the high resistance region. The higher velocities at the walls demonstrate the wall effect. The reduced flow rate at the interface of the two regions containing particles of different diameters is clearly evident.

Figures 1a, 1b, and 1c show a sequence of velocity vector fields as the inlet flow is increased in the region of high resistance. This sequence illustrates the time-dependent inlet conditions that can be described. After the initial steady state process in Figure 1a, the flow rate is increased at the top of the region of high resistance to increase the flow through this region. Due to the incompressibility the overall mass flow rate throughout the bed increases. As Figures 1b and 1c show, the increased inlet flow increases the flow rate in the bed.

As desired, Figure 1c also shows a more significant flow redistribution near the inlet, and the wall effect remains strong. The increased flow has decreased the effect of the local void minima at the interface of the two regions, though it is still evident.

CONCLUSIONS

The time-dependent Ergun equation is proposed to describe fluid flow through packed beds offering nonuniform resistance to flow. The equations lend themselves to an efficient numerical scheme making the time-dependent computation feasible. This

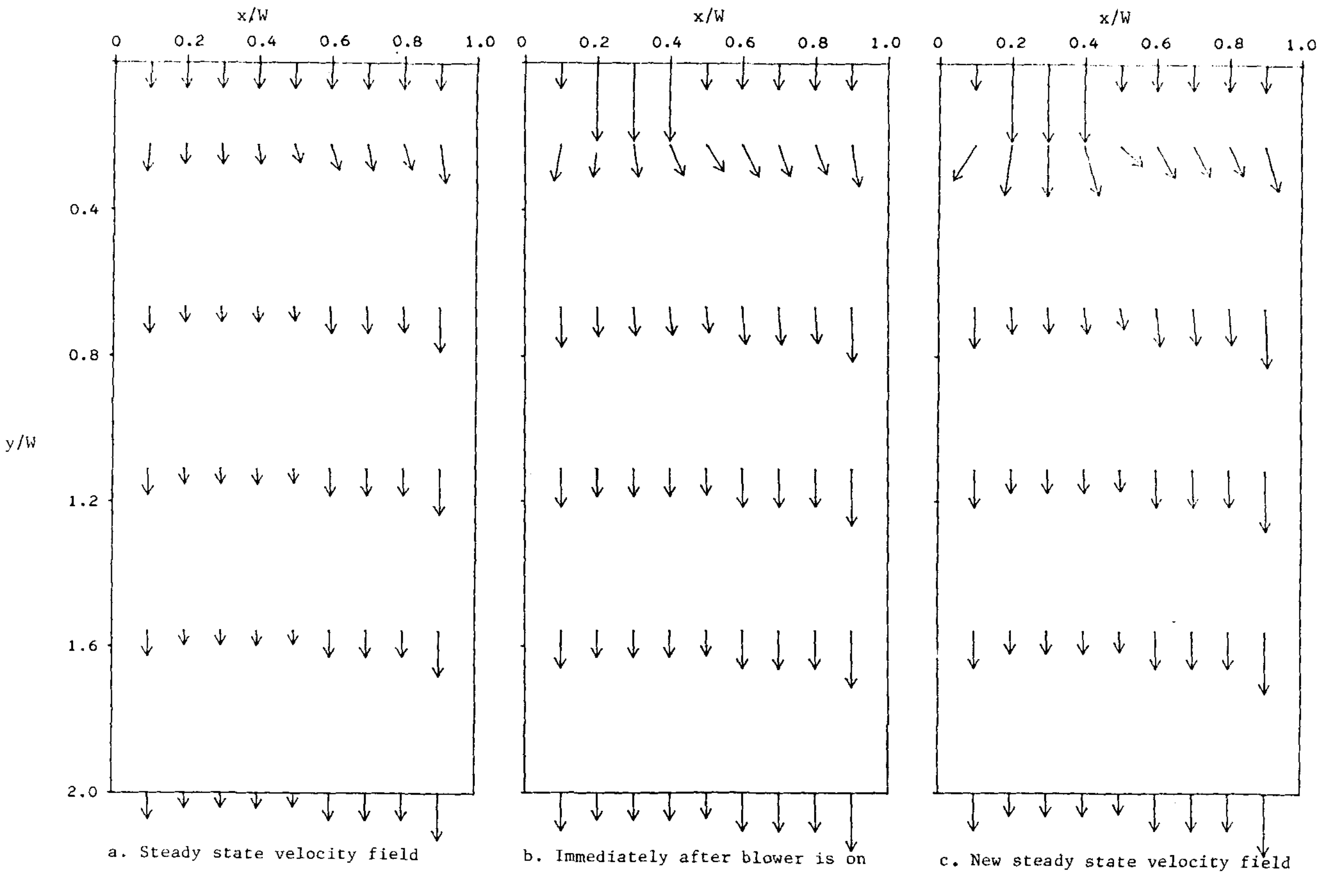

Figure 1. Time-varying sequence of computed velocity fields for parallel intercommunicating beds with ϵ = 0.38, Re_m = 39. High resistance region on left with d = 0.02 W, ϵ_{wall} = 0.47; low resistance region on the right with d = 0.04 W, ϵ_{wall} = 0.49; $\epsilon_{interface}$ = 0.365.

extension to unsteady processes coupled with an efficient numerical scheme is thought to be of considerable value, allowing the description of these processes while maintaining computational ease.

A sample of computed results is presented to exhibit some of the capabilities of this approach. They describe the steady state results that are attainable, as well as illustrating time-dependent inlet conditions designed to minimize the effect of regions of different resistance to flow.

The significance of this work is that it allows for the careful description of unsteady processes in packed beds with spatially nonuniform resistance to flow. It will facilitate the description of time-varying inlet conditions and resistance parameters that vary with time due to chemical and thermal occurrences. The work is necessary in developing a better understanding of these processes in oil shale retorts where spatial nonuniformities exist and inlet conditions are varied to improve the retort sweep efficiency by minimizing the effect of these nonuniformities. This is of major importance in developing economically feasible oil shale retorting methods.

NOTATION

d	= particle diameter
f_1	= $150\,\mu(1-\epsilon)^2/(\phi d)^2\epsilon^3$, resistance parameter
f_2	= $1.75\,\rho(1-\epsilon)/\phi d\epsilon^3$, resistance parameter
g	= gravitational vector
H	= bed height
P	= pressure
Re_m	= $\bar{V}\rho d/6\mu\,(1-\epsilon)$, modified Reynolds number
$\mathbf{V}, V, V_x, V_y$	= superficial velocity vector, its magnitude and components
$\bar{V}$	= average superficial velocity
W	= bed width

Greek Letters

ϵ	= porosity (void fraction)
λ	= iteration parameter
μ	= dynamic viscosity
ρ	= density
ϕ	= shape factor

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