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Three-Dimensional Flow of Fluids Through Nonuinform Packed Beds

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Through the statement of the Ergun equation in a vectorial form, a formulation is presented for three-dimensional flow of fluids through packed beds having a spatially variable resistance to flow. The equations were put in a form convenient for numerical solution by successive over-relaxation, and a selection of computed results is presented for cylindrical beds where the nonuniform resistance to flow obeys axial symmetry. The method outlined in the paper for calculating flow maldistribution in packed beds is thought to be a necessary first step in the representation of hot spot formation and flow nonuniformities in packed bed reactors.

SCOPE

The understanding of flow phenomena, or more specifically, flow maldistribution in packed beds having spatially nonuniform resistance to flow is of considerable practical importance in the interpretation of chemical reactor performance. In principle such flow maldistribution may occur due to spatially variable porosity or particle size distribution in the bed, or variable resistance may also be caused by radial temperature gradients in the bed. Problems of this type were discussed in two earlier papers by Stanek and Szekely (1971 and 1972) where a formulation was given by writing the axial and radial components of the Ergun equation relating pressure drop of a uniform isothermal bed to its porosity, particle diameter, and physical properties of the fluid. This procedure was shown to be only approximate by Radestock and Jeschar (1970, 1971), but the actual solution of the equations proposed by them (for two-dimensional systems) was very cumbersome.

In the present paper a statement is given of the flow problem in three dimensions by restricting the validity of the Ergun equation to an infinitesimal length of the bed and to the direction of the flow. The vectorial and differential form of the Ergun equation is then used to derive partial differential equations for the flow and pressure distributions in coordinate-free form. The handling of the equations is fully rigorous and involves no additional empiricism than that already contained in the Ergun equation. The formulation given here is thought to represent a first, necessary step for the better understanding of flow maldistribution phenomena and ultimately hot spot formation in packed bed reactors.

CONCLUSIONS AND SIGNIFICANCE

Through the statement of the Ergun equation in a differential vectorial form, equations are presented in coordinate-free form for three-dimensional fluid flow through packed beds having a distributed resistance to flow. The governing equations are developed into a form convenient for machine computation, and a selection of computed results is presented describing the velocity field and the isobar pattern in cylindrical coaxial intercommunicating beds of different resistance. Except for relatively short entrance-flow region the flow in such beds is essentially parallel (although not uniform) and a closed-form solution for the latter part is presented.

The principal significance of the work is that it provides a rigorous treatment of the Ergun equation leading to the formulation of the flow maldistribution problem as well as pressure distribution in nonuniform packings. Though strongly nonlinear, the flow equation poses no particular difficulty to the attack by numerical methods. Once the velocity pattern has been known, the pertaining pressure distribution can be obtained from a second-order partial differential equation linear in pressure also derived in the paper. All equations presented apply without a change to nonisothermal problems where heat transfer equations are coupled with the flow equations and addi-

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tional maldistribution due to nonisothermalities occurs. In such case, however, the governing equations must be supplemented by enthalpy balances in the gas and the solids. The practical significance of the work is provided by its relevant flow maldistribution problems in packed bed reactors.

Fluid flow through packed beds having a spatially nonuniform resistance to flow is of considerable practical importance in the representation of many chemical and metallurgical reaction systems. Spatial nonuniformity of resistance may be brought about by variable porosity (channeling) and also by the nonuniform distribution of the size of the solid particles that form the bed. The nonuniformities due to variable size of the solid particles may be either an undesirable effect of, for example, large particle-to-bed diameter ratio, redistribution of the particles of various diameters during filling, or, in some cases the nonuniformities are introduced intentionally to control the chemical process for example, in blast furnace operation.

In any case, the flow maldistribution that may result from such nonuniform resistance to flow could cause the formation of hot spots and loss of gas-solids contacting efficiency.

In two previous papers (1972, 1973) we have considered flow maldistribution in two-dimensional systems. For rectangular coordinates we had

$$-\frac{\partial P}{\partial x} = f_1 V_x + f_2 V_x \cdot |V_x| \qquad (1a)$$

for the direction of flow, and

$$-\frac{\partial P}{\partial y} = f_1 V_y + f_2 V_y \cdot |V_y| \qquad (1b)$$

for the transverse direction.

However, Jeschar and Radestock (1969) have suggested that such an approach is formally incorrect because Equations (1a) and (1b) are not invariant to the transformation of the coordinates and the resulting streamlines would not be generally perpendicular to the isobars. A close examination of the results derived from Equations (1a) and (1b) has revealed that little error is introduced in using this approach provided the flow field is largely parallel; this condition was observed in the cases discussed in our previous two papers (1972, 1973); thus the findings reported there remain valid.

A more rigorous approach would be to write the differential form of the Ergun equation in vector notation, thus

$$-\nabla P = \mathbf{V}(f_1 + f_2 V) \qquad (2)$$

Equation (2), in effect, is the Ergun equation with the validity confined to an infinitesimal length of the bed and to the direction of flow, which in general is different from that of the bed axis.

For a compressible fluid it is more convenient to work with the mass velocity of the fluid. Assuming the fluid to obey the equation of state, one obtains without any restriction of the validity:

$$-\nabla(P^2) = \mathbf{G}\,(g_1 + g_2 G) \qquad (3)$$

Under steady state Equation (3) can be rearranged to give an expression which does not contain the mass velocity

$$\nabla^2(P^2) - \nabla(P^2) \bullet \nabla\,[\ln(g_1/2 + \sqrt{(g_1/2)^2 + g_2\,|\nabla(P^2)|})] = 0 \qquad (4a)$$

An analogous expression for an incompressible fluid is

$$\nabla^2 P - \nabla P \bullet \nabla\,[\ln(f_1/2 + \sqrt{(f_1/2)^2 + f_2\,|\nabla P|})] = 0 \qquad (4b)$$

The symbols $|\nabla(P^2)|$ and $|\nabla P|$ designate the magnitudes of the vectors $\nabla(P^2)$ and ∇P, respectively.

Radestock and Jeschar (1969, 1970, 1971a, 1971b) used expressions analogous to Equations (4a) and (4b) to solve some two-dimensional problems in packed beds. A major practical disadvantage of this approach was the fact that a very large number of iterations (about 5000) were required to solve the governing equations by successive relaxation. It would appear, therefore, that the use of this technique for solving three-dimensional problems would require excessive computer time.

The purpose of the work described in this paper is to develop a formulation which is more amenable to solution by numerical techniques.

FORMULATION

Let us consider a general, three-dimensional fluid flow field in a packed bed where the resistance to flow may be spatially dependent. Equations (2) and (3) will form the starting point of our development.

Incompressible Fluids

Let us use the operator $\nabla\times$ on Equation (2) to obtain

$$\nabla \times \mathbf{V} - \mathbf{V} \times \nabla\,[\ln(f_1 + f_2 V)] = 0 \qquad (5)$$

which is a vector equation containing **V**, the velocity vector as the only dependent variable.

The components of the velocity vector also have to satisfy the equation of continuity, thus

$$\nabla \bullet \mathbf{V} = 0 \qquad (6)$$

Upon finding the velocity field through the solution of Equations (5) and (6), the pressure distribution may then be evaluated from

$$\nabla^2 P = -\mathbf{V} \bullet \nabla\,(f_1 + f_2 V) \qquad (7)$$

It should be readily apparent that the use of Equation (7) is preferable to the previously given Equation (4b) because it is linear in pressure; once the velocity field is known, the right-hand side of Equation (7) is a known function of the spatial coordinates.

It may be of interest to note that the rate of energy dissipation may be obtained from Equation (2) by forming scalar product with the velocity vector.

On combining the result with Equation (6) we have

$$\nabla \bullet (\mathbf{V}\,P) = -\,(f_1 V^2 + f_2 V^3) \qquad (8a)$$

On applying the Gauss-Ostrogradsky theorem and integrating over a volume θ closed by the surface φ we obtain

$$-\iint_{\varphi} P\,\mathbf{V} \bullet d\boldsymbol{\varphi} = \iiint_{\theta} (f_1 V^2 + f_2 V^3)\,d\theta \qquad (8b)$$

The left-hand side represents the net rate of input of pressure energy supplied into the volume θ; the right-hand side expresses the net rate of energy dissipation in the same volume.

Compressible Fluids

On following an analogous procedure described in the preceding section dealing with incompressible fluids, we obtain the following equation from Equation (3) in terms of mass velocity suitable for solving the mass velocity field

$$\nabla \times \mathbf{G} - \mathbf{G} \times \nabla\, (\ln(g_1 + g_2G)) = 0 \qquad (9)$$

Again, once the velocity field is known through the solution of Equation (9) for the appropriate boundary conditions, the pressure field or the isobars may then be computed from

$$\nabla^2(P^2) = -\,(g_1 + g_2G)\, \nabla \bullet \mathbf{G} - \mathbf{G} \bullet \nabla\, (g_1 + g_2G) \qquad (10a)$$

For steady state conditions Equation (10a) may be simplified with the aid of the equation of continuity to obtain:

$$\nabla^2(P^2) = -\,\mathbf{G} \bullet \nabla\, (g_1 + g_2G) \qquad (10b)$$

since

$$\nabla \bullet \mathbf{G} = \nabla \bullet (\rho\, \mathbf{V}) = -\,\epsilon \frac{\partial \rho}{\partial t} = 0 \qquad (11)$$

The mechanical energy balance may then be obtained by forming the scalar product of Equation (3) and the velocity vector. On using the steady state form of the continuity equation, after some manipulation, we obtain

$$-\,\nabla \bullet (\mathbf{V}\, P) = \frac{1}{2\, P\, \rho}\, (g_1G^2 + g_2G^3) + \frac{P}{\rho^2}\, \mathbf{G} \bullet \nabla \rho \qquad (12a)$$

which may be written as

$$-\,\nabla \bullet (\mathbf{V}\, P) = \frac{\rho}{2\, P}\, (g_1V^2 + g_2\, \rho\, V^3) - P\, \nabla \bullet \mathbf{V} \qquad (12b)$$

Equations (12a) and (12b) when applied again in their integral form to a volume θ express the fact that the pressure energy supplied into this volume through its surface φ, at a rate given by the left-hand side is partially dissipated (the first term on the right-hand side of Equation (12a) or (12b) is the rate of dissipation per unit volume) and partially converted reversibly into internal energy (the second term on the right-hand side is the net rate of conversion per unit volume).

However, for the steady and isothermal flow the left-hand side of Equations (12a) and (12b) equals zero in order to satisfy continuity and the whole dissipation is balanced by the loss of internal energy of the gas (the second right-hand side term).

Simplifying Assumptions, Asymptotic Regimes

The previously given Equations (5) to (12), together with the appropriate boundary conditions, represent a complete statement of the problem for isothermal systems. In nonisothermal systems the parameters f_1, f_2, g_1, g_2 become temperature-dependent and the set of equations must be supplemented by the enthalpy balances in the fluid and the solids. Before proceeding with the specific description of particular geometries, it is desirable to examine possible simplifying assumptions.

The formulations of both the incompressible and compressible flow problems contain two parameters each, the relative importance of which may be assessed from

$$V_0\, f_2/f_1 = G_0\, g_2/g_1 = 7.10^{-2}Re, \quad \text{where} \quad Re = \frac{V_0 \rho}{a \mu} \qquad (13)$$

It is seen that when $Re \geqq 150$ the turbulent dissipation predominates and the viscous contribution amounts to less than 10%; in contrast when $Re \leqq 1.5$, viscous dissipation predominates and the turbulent contribution amounts to less than 10%. When $1.5 \leqq Re \leqq 150$, both these effects have to be taken into consideration.

$Re > 150$

This is the case of major practical interest. Equation (5) then simplifies to

$$\nabla \times \mathbf{V} - \mathbf{V} \times \nabla\, (\ln(f_2V)) = 0 \qquad (14)$$

Equation (14) has some important features which deserve special attention:

(i) When put in dimensionless form using some average velocity V_0 and a characteristic dimension of the system, the dimensionless form will be formally unchanged. Its solution would thus be valid for any arbitrary velocity V_0 in systems with similar geometry.

This gives Equation (14) a rather broad applicability.

(ii) Since the parameter f_2 characterizing the resistance of the packing appears in Equation (14) as a natural logarithm, the function giving its spatial distribution may be scaled by an arbitrary factor, for example $(f_2)_0$, and the solution would then apply to the whole family of problems with similar geometry but different scaling factors.

A simplified version of Equation (7), governing the pressure distribution, is

$$\nabla^2 P = -\,\mathbf{V} \bullet \nabla\, (f_2V) \qquad (15)$$

This equation can be rendered dimensionless by means of the parameters V_0, $(f_2)_0$, and R. From the dimensionless form one can infer that the pressure difference between the inlet and the outlet of the bed may be written as

$$P_{\text{inlet}} - P_{\text{outlet}} = k(f_2)_0V_0^2R \qquad (16)$$

where the constant k depends on the distribution of the relative local resistance f_2. Furthermore, one can say that on defining V_0 as the mean velocity in the bed and $(f_2)_0$ as the integral average of f_2, the magnitude of the constant k will be of the order of Z/R.

$Re < 1.5$

Under these conditions Equation (5) may be written as

$$\nabla \times \mathbf{V} - \mathbf{V} \times \nabla\, (\ln(f_1)) = 0 \qquad (17)$$

In some cases it may be more convenient to solve directly the pressure distribution:

$$\nabla^2 P - \nabla \bullet \nabla\, (\ln(f_1)) = 0 \qquad (18)$$

We note that the developments described here for incompressible fluids through the statement of Equations (14) to (18) may be readily extended to compressible fluids by replacing f_1, f_2, $(f_2)_0$, $\mathbf{V}$, V_0 and P, by g_1, g_2, $(g_2)_0$, $\mathbf{G}$, G_0 and P^2, respectively.

TWO-DIMENSIONAL PROBLEMS

Parallel Flow in a Cylindrical Bed with Axial Symmetry

Let us consider parallel flow in a cylindrical system where the nonuniformity of the packing exhibits cylindrical symmetry and where the inlet and outlet conditions are also symmetrical.

For the cylindrical coordinate system the components of some of the vector operators may be written as

$$\nabla\, s = \mathbf{e}_r \frac{\partial s}{\partial r} + \mathbf{e}_\Phi \frac{1}{r} \frac{\partial s}{\partial \Phi} + \mathbf{e}_z \frac{\partial s}{\partial z} \qquad (19)$$

$$\nabla \times \mathbf{w} = \mathbf{e}_r \left[\frac{1}{r} \frac{\partial w_z}{\partial \Phi} - \frac{\partial w_\Phi}{\partial z} \right] + \mathbf{e}_\Phi \left[\frac{\partial w_r}{\partial z} - \frac{\partial w_z}{\partial r} \right] + \mathbf{e}_z \left[\frac{1}{r} \frac{\partial (r\, w_\Phi)}{\partial r} - \frac{1}{r} \frac{\partial w_r}{\partial \Phi} \right] \qquad (20)$$

For incompressible flow through a cylindrical bed with axial symmetry (that is, $\partial/\partial\Phi = 0$ and $V_\Phi = 0$) and substitution from Equations (19) and (20) into Equation (5) yields the following:

$$\frac{\partial V_r}{\partial z} - \frac{\partial V_z}{\partial r} + V_r \frac{\partial \ln(f_1 + f_2 V)}{\partial z} - V_z \frac{\partial \ln(f_1 + f_2 V)}{\partial r} = 0 \quad (21)$$

In general Equation (21) has to be solved numerically; analytical solutions do exist, however, for the special case when $\partial f_1/\partial z = \partial f_2/\partial z = 0$, when the resistance does not vary in the direction of flow. If the bed is sufficiently long, all radial components of the velocity vanish and the flow becomes parallel. On putting $V_r = 0$ and $V = V_z$, Equation (21) is readily solved to obtain

$$V_z = -(f_1/2f_2) + \sqrt{(f_1/2f_2)^2 + k/f_2} \quad (22)$$

The integration constant k is determined from an overall balance on the gas.

$$V_0 R^2 = \int_0^R 2r\, V_z dr = \int_0^R 2r\, [-f_1/2f_2 + \sqrt{(f_1/2f_2)^2 + k/f_2}]\, dr \quad (23)$$

which can be solved explicitly if f_1 and f_2 are known functions of the radius. When $f_1 = 0$ the solution takes the following form:

$$V_z = V_0\, f_2^{-0.5}/(f_2^{-0.5})_0, \quad \text{where} \quad (f_2^{-0.5})_0 = \frac{2}{R^2} \int_0^R \frac{r\, dr}{f_2^{0.5}} \quad (24a, b)$$

When $f_2 = 0$, we have

$$V_z = V_0 f_1^{-1}/(f_1^{-1})_0, \quad \text{where} \quad (f_1^{-1})_0 = \frac{2}{R^2} \int_0^R \frac{r\, dr}{f_1} \quad (25a, b)$$

Two-Dimensional, Nonparallel Flow in a Cylindrical Bed with Axial Symmetry

In many systems exhibiting flow maldistribution, the flow field is nonparallel. Let us consider a system where the viscous dissipation terms may be neglected ($Re > 150$). Under these conditions Equation (21) may be rewritten to obtain the following:

$$\frac{\partial V_r}{\partial z} - \frac{\partial V_z}{\partial r} + V_r \frac{\partial \ln f_2}{\partial z} - V_z \frac{\partial \ln f_2}{\partial r} + \frac{1}{V^2}\left[V_r \left(V_z \frac{\partial V_z}{\partial z} + V_r \frac{\partial V_r}{\partial z} \right) - V_z \left(V_z \frac{\partial V_z}{\partial r} + V_r \frac{\partial V_r}{\partial r} \right) \right] = 0 \quad (26)$$

The components of the velocity vector V_r, V_z have to satisfy the continuity equation; this condition is readily met by introducing ψ, the stream function defined as

$$V_z = -\frac{1}{r} \frac{\partial \psi}{\partial r} \quad \text{and} \quad V_r = \frac{1}{r} \frac{\partial \psi}{\partial z} \quad (27a, b)$$

Upon recasting Equation (27) in terms of the stream function we have

$$\frac{\partial^2 \psi}{\partial r^2}\left[2\left(\frac{\partial \psi}{\partial r}\right)^2 + \left(\frac{\partial \psi}{\partial z}\right)^2 \right] + \frac{\partial^2 \psi}{\partial z^2}\left[2\left(\frac{\partial \psi}{\partial z}\right)^2 + \left(\frac{\partial \psi}{\partial r}\right)^2 \right]$$

(continued)

$$+ \left[\left(\frac{\partial \psi}{\partial r}\right)^2 + \left(\frac{\partial \psi}{\partial z}\right)^2 \right] \left[\frac{\partial \psi}{\partial z} \frac{\partial \ln f_2}{\partial z} + \frac{\partial \psi}{\partial r}\left(\frac{\partial \ln f_2}{\partial r} - \frac{2}{r} \right) \right] + 2 \frac{\partial^2 \psi}{\partial r \partial z} \frac{\partial \psi}{\partial r} \frac{\partial \psi}{\partial z} = 0 \quad (28)$$

Before proceeding further we note again that Equation (28) remains formally unchanged if rendered dimensionless by means of the mean velocity, V_0 [defined in Equation (23)] and the column radius R. The new dimensionless variables are distinguished from the corresponding dimensional variables by asterisks.

In order to solve Equation (28) by some numerical technique, the boundary conditions have to be specified at the following locations:

(i) at the wall of the column ($r^* = 1$; $0 < z^* < Z/R$),
(ii) at the axis of the column ($r^* = 0$; $0 < z^* < Z/R$),
(iii) at the inlet of the bed ($z^* = 0$; $0 < r^* < 1$), and
(iv) at the outlet of the bed ($z^* = Z/R$; $0 < r^* < 1$).

The wall of the column is impervious to gas and the stream function must therefore remain constant along $r^* = 1$. The symmetry condition is formally identical to the imperviousness and thus the stream function at the axis must also remain constant. Since the introduction of the stream function increases the order of the governing differential equation, one of the constants is arbitrary. We choose for numerical reasons $\psi^* = 0$ at $r^* = 0$ (all z^*). The value at the wall is set equal to $\psi^* = -0.5$ which makes the dimensionless flow rate in each column cross section equal unity.

The condition at the inlet has to specify the way in which the gas is introduced into the bed. We may either assume that gas is supplied uniformly over the inlet so that $V_z = V_0$ ($z^* = 0$; $0 < r^* < 1$) and the stream function at the inlet is then given by

$$\psi^* = \psi/V_0 R^2 = -r^{*2}/2, \quad z^* = 0 \quad (29a)$$

Alternatively we may require that the pressure be constant over the inlet surface which mandates $\partial P/\partial r = 0$, from which $V_r = 0$, and from which with the aid of Equation (27b) we have

$$\frac{\partial \psi^*}{\partial z^*} = 0, \quad z^* = 0 \quad (29b)$$

For the outlet end we specify that the pressure is constant and thus we have a condition similar to Equation (29b) at the point $z^* = Z/R$.

Through the preceding Equations (5) to (29) we developed a general formulation for nonuniform flow through packed beds and illustrated how this general development may be written in a form convenient for computation for specific conditions and geometries. Let us conclude this presentation by the discussion of some computed results.

COMPUTED RESULTS

The computed results to be given here concern intercommunicating coaxial beds each having a different resistance to flow at high Reynolds numbers. The systems to be considered are sketched in Figures 1a and 1b, where it is seen that the core of the bed is filled with a packing which has a different resistance to flow than the material contained in the outer shell. The radius of the core was taken as $R/2$ and the height of the column was taken to be the same as its length, so that $Z/R = 1$.

Two specific cases were considered:

(a) When the resistance in the core is 4 times smaller than in the rest of the bed,
(b) When the resistance in the core is 4 times larger than in the rest of the bed.

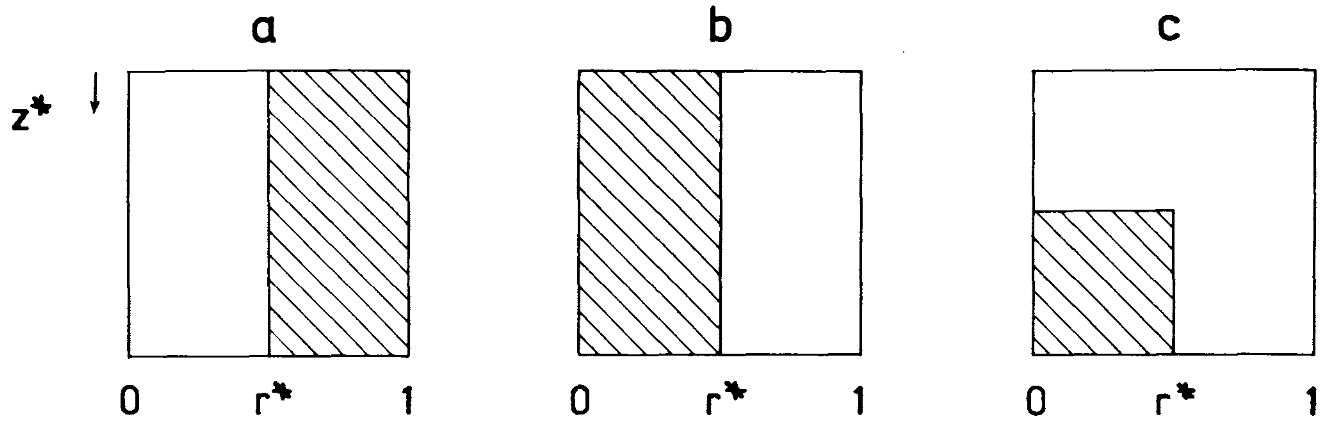

Fig. 1. Sketch of bed nonuniformities examined in the paper. (The shaded area indicates section of resistance four times that in the rest of the bed).

TABLE 1. THE MAXIMUM RELATIVE DEVIATION OF THE STREAM FUNCTION (%) IN VARIOUS STAGES OF ITERATION

	Case a			Case b		
No. of iterations	$\alpha = 1.2$	$\alpha = 1.3$	$\alpha = 1.4$	$\alpha = 1.2$	$\alpha = 1.3$	$\alpha = 1.4$
10	2.8930	2.6841	3.1473	3.8942	3.8055	4.5026
20	0.6407	0.4409	0.4938	0.8288	0.7815	0.5103
25	0.3210	0.1876	0.1962	0.3496	0.1579	0.1439
30	0.1625	0.0804	0.0770	0.1445	0.0512	0.0392
35	0.0824	0.0346	0.0302	0.0592	0.0164	0.0106
36	0.0720	0.0292	0.0251	0.0496	0.0132	0.0080
38	0.0550	0.0210	0.0172	0.0346	0.0084	—
40	0.0420	0.0148	0.0117	0.0241	—	—
41	0.0366	0.0126	0.0097	0.0202	—	—
43	0.0280	0.0091	—	0.0141	—	—
45	0.0214	—	—	0.0098	—	—
51	0.0095	—	—	—	—	—

The values of f_2 were in both cases scaled so as to make the integral average value of f_2 equal unity $(f_2)_0 = 1$. We note that f_2, the resistance parameter, would be increased by a factor of four due to a local decrease in the particle diameter by the same factor; a similar change in f_2 could also be brought about by decreasing the local porosity, for example, from 0.5 to 0.345. The boundary conditions used corresponded to Equation (29a) that is, a uniform approach velocity to the bed was assumed.

For the purpose of computation Equation (28) was put in a finite difference form and the resultant equations were solved by successive overrelaxation. The computational grid contained 11 × 11 points and the actual course of the computational procedure is illustrated in Table 1 which summarizes the absolute values of the maximum deviation (in %) at several stages of the iteration for three values of the overrelaxation factor. It is seen that the number of iterations is quite acceptable so that the computational scheme outlined here seems quite attractive.

Figure 2 shows the streamline pattern corresponding to case (b) defined in Figure 1 previously. The figure shows the region of redistribution where the streamlines are nonparallel to be rather short even though the relative length of the bed is small ($Z/R = 1$). Similar situation was observed on numerical results of case(a) not shown graphically. The fractional flow rate of gas within the radius $r^* = 0.5$ at the bed exit was found equal 0.378 and 0.150 for cases (a) and (b), respectively. Corresponding values of the fractional flow rates for parallel flow following from Equations (24a) and (24b) are 0.400 and 0.143. The differences are mainly due to approximate character of the numerical routine.

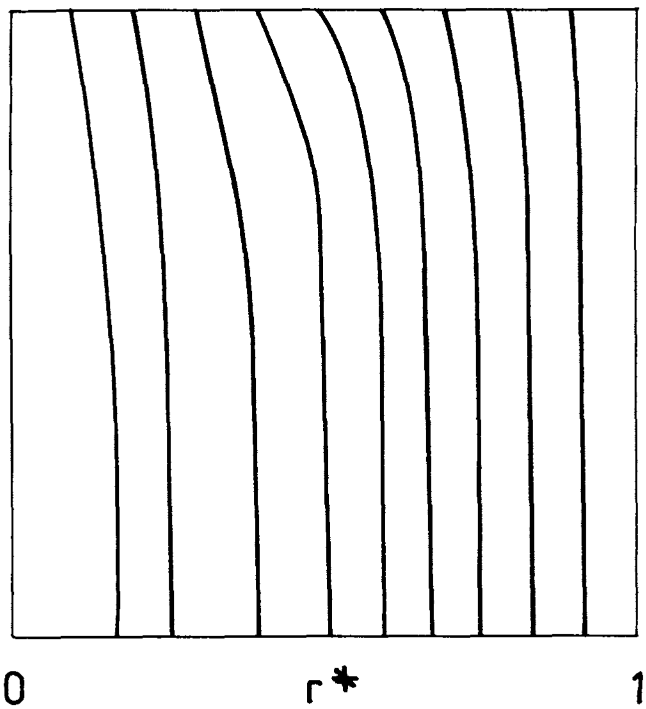

Fig. 2. Computed streamlines for case b of Figure 1.

The isobars, corresponding to the streamline pattern shown in Figure 2 are given in Figure 3. It is seen that the pressure shows marked variations at the inlet; this behavior is a direct consequence of the uniform inlet velocity that was specified in the boundary condition.

The integral mean value of the inlet pressure (the outlet pressure has been set at zero, arbitrarily), given in its dimensionless form as

$$(P^*_{\text{inlet}})_0 = (P_{\text{inlet}}/(f_2)_0 R V_0^2)_0$$

was found to have quite close values of 0.905 and 0.909 for cases (a) and (b), respectively.

In the type of nonuniform beds discussed here, there will exist a finite radial velocity. Figure 4 shows the contours of the constant radial component of the velocity vector. Expectedly, markedly nonzero values of radial velocity exist only near the inlet.

Had we used the other boundary condition, stipulating a constant pressure at the inlet [Equation (29b)], the solution would have been much easier. In fact an analytical

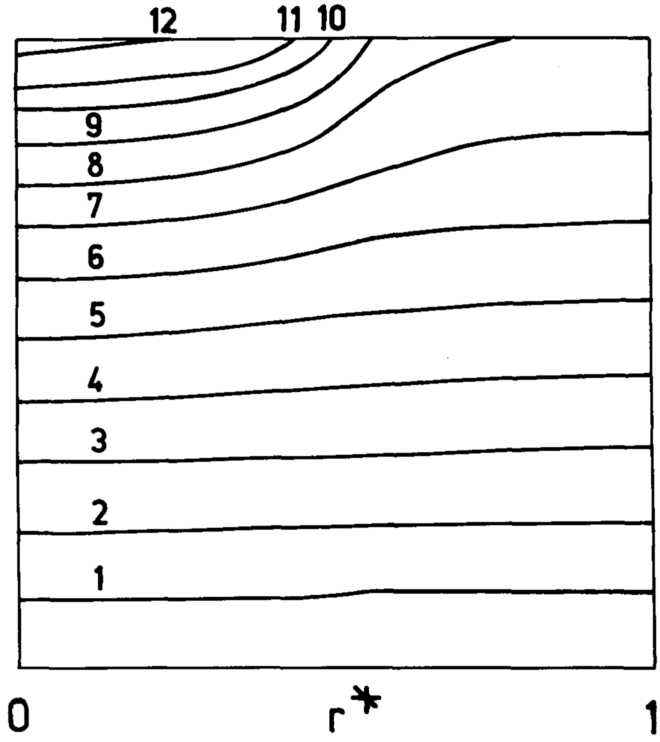

Fig. 3. Computed isobars for Case b of Figure 1. (The isobars 1, 2, 3, etc. correspond to the dimensionless pressure 0.1, 0.2, 0.3, etc.)

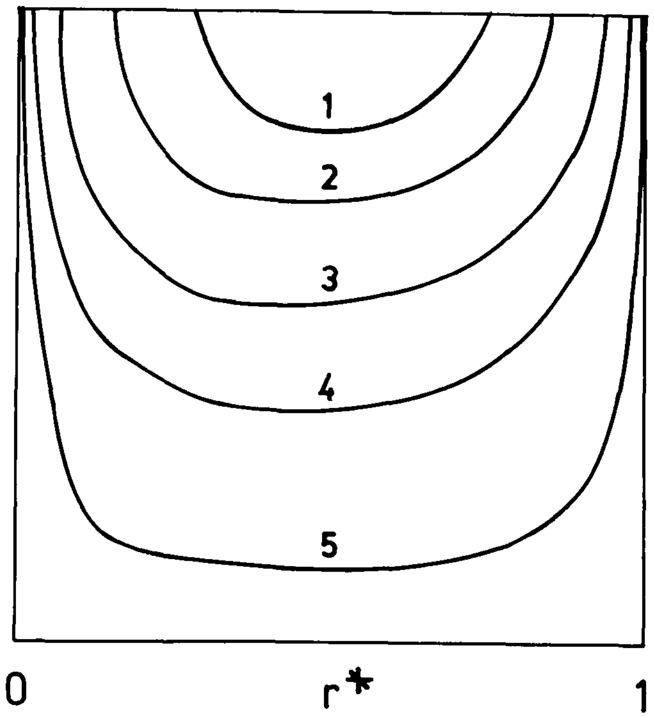

Fig. 4. Computed contours of constant radial velocity V_r^* for Case b of Figure 1. (The contours 1, 2, 3, 4, 5 correspond to V_r^* equal 0.2, 0.1, 0.04, 0.015, 0.002, respectively.)

solution would have been available as given by Equations (24a) and (24b). The streamline pattern would have been parallel flow and the isobars evenly spaced straight lines perpendicular to the streamlines. The inlet pressure (now uniform) could then be computed from

$$P^*_{\text{inlet}} - P^*_{\text{outlet}} = (f_2^{-0.5})_0^{-2}/(f_2)_0 \cdot (Z/R) \quad (30)$$

The right-hand side of the last equation, which is identical to the constant k in Equation (16), would have the numerical value of 0.788 and 0.746 for cases (a) and (b), respectively. From here it follows that a nonuniform bed under parallel flow would display generally lower pressure drop than corresponding uniform bed of identical length V_0 and integral average resistance $(f_2)_0$ because for nonuniform beds $(f_2^{-0.5})_0^{-2} < (f_2)_0$.

The apparently marked effect of the inlet conditions on the streamlines and isobars requires further comment. It must be noted, however, that the overall relationship between pressure drop and the flow rate through a nonuniform bed is much less affected by the inlet conditions. Moreover, the effects of the inlet conditions are thought to be more marked for the relatively short beds that are considered here. It is stressed that experimental information would be desirable to provide a more satisfactory definition of the inlet conditions.

Some insight may be obtained into this problem, however, by considering the flow system sketched in Figure 1c and evaluating the isobars for both uniform inlet pressure and uniform inlet velocity. The computed isobars are shown in Figures 5 and 6, respectively. The computed dimensionless inlet pressures are $P^*_{\text{inlet}} = 0.905$ and $(P^*_{\text{inlet}})_0 = 0.912$ for these two cases, respectively.

The numerically computed values of the pressure and of the stream function at the level $z^* = 0.5\ Z/R$ and $0 < r^* < 1$ indicate that neither of these inlet boundary conditions [that is, (29a) or (29b)] is satisfied and thus the real situation must be an intermediate between these two limits.

A further comment may be appropriate on the computation of the pressure distribution. Having found the streamline field one may be tempted to use one component of Equation (2) directly in the principal direction of the flow, for the z direction (neglecting f_1) for example,

$$-\frac{\partial P}{\partial z} = V_z f_2 \sqrt{V_z^2 + V_r^2} \quad (31)$$

to compute the pressure field since this does not require an iterative procedure. The experience shows, however, that such results are not consistent with those obtained by integrating in the other direction. Moreover, the results may be even physically unacceptable in some cases. These difficulties are avoided by using Equation (15) which

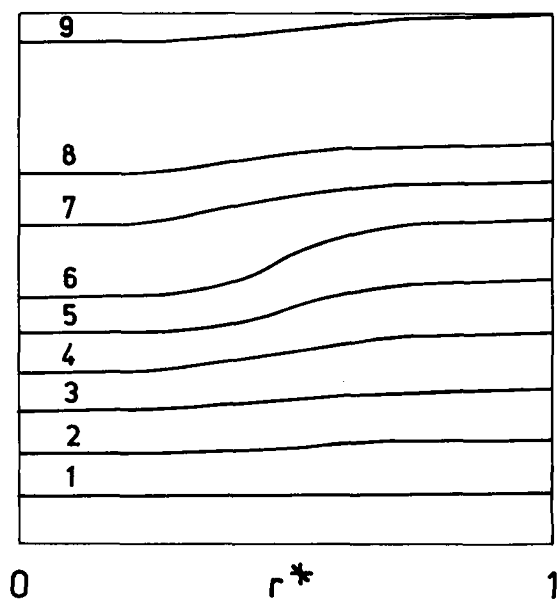

Fig. 5. Computed isobars for case c of Figure 1 at uniform inlet pressure. (The numbers on the isobars have the same meaning as in Figure 3.)

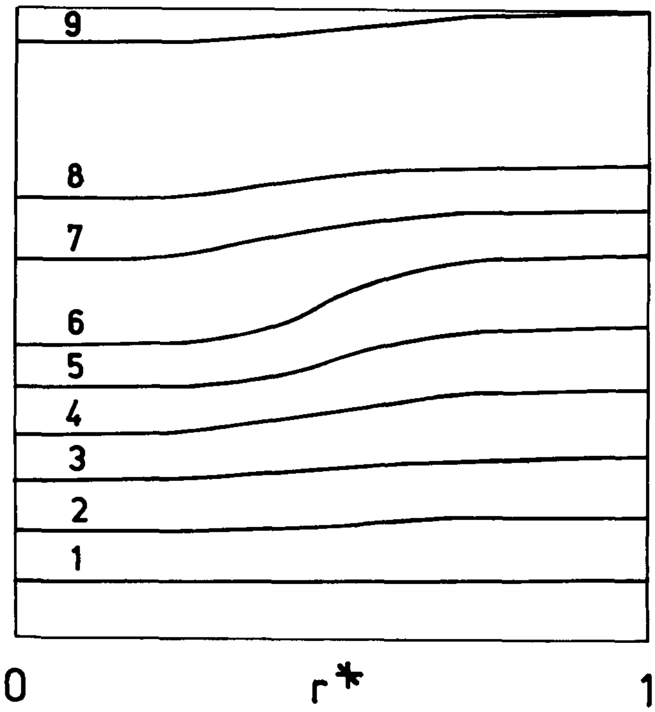

Fig. 6. Computed isobars for case c of Figure 1 at uniform feed to the bed.

being of second order requires two boundary conditions.

One boundary condition may usually be provided by setting the outlet pressure at the background level (usually zero), this will make the outlet line $z^* = Z/R$ $(0 < r^* < 1)$ an isobar. With a constant outlet pressure, the inlet pressure is no longer an independently adjustable variable because it has to be consistent with both the inlet boundary condition imposed on the flow equation and with the condition specified through the overall pressure drop. The safest way seems to be to stipulate the inlet pressure gradient which can be easily computed from the known stream function and the distribution of the resistance at the inlet.

CONCLUSIONS

A formulation is developed describing three-dimensional fluid flow through packed beds offering nonuniform resistance to flow. The problem is stated by writing the vectorial form of the Ergun equation and this representation is thought to be more rigorous than previously published relationships which were shown to be only approximate in recent publications by Jeschar.

The governing equations were manipulated into a form which was very convenient for solution by numerical methods and the computational procedure adopted was found to converge quite rapidly. This transformation of the vectorial form of the Ergun equation is thought to represent a major advance over the published work of Jeschar et al., the solution of whose equations even in two dimensions required excessive computer time.

A series of computed results are also presented describing flow maldistribution in terms of velocity profiles and isobar patterns for cylindrical beds where the variability of the resistance to flow exhibits axial symmetry.

It is thought that the significance of the paper lies in providing a rigorous formulation for flow in packed beds with spatially nonuniform resistance together with an efficient computational procedure for solving the resultant equations. The work described here represents a necessary step in the better understanding of flow maldistribution in packed bed reactors where spatially variable resistance to flow may be brought about by both variable porosity and variable temperatures. These flow maldistribution phenomena are thought to play a major role in the formation of hot spots and possibly instabilities in the operation of packed bed reactors.

NOTATION

a = specific surface of packing
d = particle diameter
$\mathbf{e}_r, \mathbf{e}_\Phi, \mathbf{e}_z$ = unit vectors
f_1 = $150\mu(1-\epsilon)^2/d^2\epsilon^3$ parameter of resistance
f_2 = $1.75\rho(1-\epsilon)/d\epsilon^3$ parameter of resistance
$\mathbf{G}, G$ = mass velocity vector and its magnitude
G_0 = average superficial mass velocity in the bed
g_1 = $300(1-\epsilon)^2P\mu/\rho\, d^2\epsilon^3$ parameter of resistance
g_2 = $3.5(1-\epsilon)P/\rho\, d\epsilon^3$ parameter of resistance
k = constant
P, P^* = $P/(f_2)_0V_0^2R$ dimensional, dimensionless pressure
R = column radius
r, r^* = r/R dimensional, dimensionless radial coordinate
Re = Reynolds number defined in Equation (13)
s = scalar quantity
t = time
$\mathbf{V}, V, V_x, V_y, V_r, V_z, V_\Phi$ = superficial velocity vector, its magnitude and components
V_0 = average superficial velocity in the bed defined in Equation (23)
$\mathbf{w}, w_r, w_z, w_\Phi$ = vector quantity and its components
x, y = rectangular coordinates
z, z^* = z/R dimensional, dimensionless coordinate of height measured from bed inlet
Z = bed depth

Greek Letters

α = overrelaxation factor
ϵ = porosity (void fraction)
Φ = cylindrical coordinate of angle
μ = dynamic viscosity
ψ, ψ^* = ψ/V_0R^2 dimensional, dimensionless stream function
ρ = density
φ = surface
θ = volume

Subscript

0 = average quantity

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