A New Model for Granular Porous Media:

Part I. Model Formulation

A new model for porous media comprised of monosized, or nearly monosized grains, is developed. In applying this model to a packed bed, the bed is assumed to consist of a series of statistically identical unit bed elements each of which in turn consists of a number of unit cells connected in parallel. Each unit cell resembles a piece of constricted tube with dimensions which are random variables. The problem of flow through each unit cell is reduced, subject to reasonable assumptions, to the determination of the flow in an infinitely long periodically constricted tube. The solution of this flow problem is given in a companion publication. This model, together with the solution of the flow through it, can be used for the modeling of processes which take place in the void space of a bed.

As a preliminary test, theoretical friction factor values, based on the proposed model, were compared with experimental ones for two different beds and found to be in good agreement even in the region of high Reynolds numbers where the nonlinear inertia terms are significant.

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SCOPE

The main purpose of this paper is to present a new model for porous media of the type represented by randomly packed beds of monosized, or nearly monosized, grains. The model has been developed as a first step in the study of filtration of suspensions through packed beds (commonly encountered in water and waste water treatment), and its immediate objective is to provide a basis for the prediction of the deposition rate of particulate matter and the attendant increase in pressure drop, which is caused by the accumulation of deposited matter in the interstitial spaces. In addition, the proposed model should be of value in the modeling of any process taking place in a granular porous medium, which is relatively more strongly influenced by the nature of the void space of the porous medium than by that of the solid matrix. As a preliminary model validation, the model has been used to obtain the relationship of the friction factor versus the Reynolds number of a packed bed of the type described above.

The development of the model presented herein is necessitated by the failure of existing porous media models in explaining and predicting the major phenomena associated with the deep bed filtration process. Capillary models are found to be totally inadequate in the estimation of the filtration rate mainly because of the omission of the curvature effect in assumed Poiseuille flow, which is believed to be of significance in the deposition process of the particulate matter. As a consequence, the filtration coefficient obtained from trajectory calculations based on capillary models is several orders of magnitude less than that observed in experiments (Payatakes, 1972). Several previous investigators have employed the single collector concept in the study of deep bed filtration (Yao et al., 1971; Spielman and Goren, 1970). The single collector concept assumes that the porous medium is equivalent to an assembly of independent bodies of simple geometry. However, because of the inherent limitation that the grains (or collectors) are considered to be independent, the effect of the neighboring grains on each other cannot be dealt with, which in turn results in failure to predict the pressure drop increase resulting from the deposition of particulate matter. Furthermore, these studies fail to give accurate predictions when the sizes of the particles to be filtered are substantially greater than 2μ. The filtration model proposed by FitzPatrick (1972) which utilizes the packed bed model developed by Happel (1959) represents an improvement in the area of single collector models since it accounts, to a certain extent, for the presence of neighboring grains, but in the opinion of the authors it is not equipped to deal with the filtration of large particles. It is also not well suited for prediction of the effect of deposited matter on either the value of the filter coefficient or the increase of pressure drop.

The basic flow channel considered in this new model is that of a constricted tube formed by the surface of neighboring grains. Thus, the three important factors concerning the filtration process—effect of neighboring grains, curvature effect, and the convergent-divergent nature of flow channel—are included in the model which is believed to be better suited for further studies in deep bed filtration.

CONCLUSIONS AND SIGNIFICANCE

A new model of the void space in randomly packed beds of monosized, or nearly monosized, grains has been developed. According to this model, a bed is divided into a series of statistically identical unit bed elements, any one of which can be used for describing the entire bed. Each unit bed element consists of a number of unit cells connected in parallel and each unit cell resembles a piece of constricted tube. The unit cells within a unit bed element are not, in general, equal to each other. A number of different types of unit cells are considered. Unit cells belong-

ing to different types are unequal but geometrically similar. The geometry of all unit cells can be uniquely determined from the following readily obtainable experimental information: grain size distribution, porosity, and saturation versus capillary pressure data. The model can be used to study the flow of fluids through granular randomly packed beds. It is shown that this problem can be reduced, subject to reasonable assumptions, to the determination of the flow in a single infinitely long periodically constricted tube, the geometry of which is connected to that of the unit cells. The solution of this problem is given in a companion publication. Based on this solution, it is shown that the friction factor of granular randomly packed beds can be calculated as a function of the superficial Reynolds number even in the region of intermediate Reynolds values where the nonlinear inertia effects are not negligible. It is shown that, in the important case of low Reynolds numbers, the friction factor is given by the product of $(N_{Re})_s^{-1}$ and two other factors. The first of these factors is completely determined from geometric characteristics of the bed, while the other being of hydrodynamic nature, can be calculated numerically. An approximate analytical expression is given which allows the calculation of the hydrodynamic factor. This expression has been obtained by interpolation of the calculated values of the hydrodynamic factor for several characteristic unit cell geometries. Experimental and theoretical friction factor relations for two different packed beds were compared and found in satisfactory agreement.

The model of the void space coupled with the solution of the flow through its unit cells can form the basis for the study of processes taking place in granular randomly packed beds, which are more influenced by the nature of the void space of the bed rather than by that of the solid matrix. Such a process is, for example, the deep bed filtration commonly encountered in waste water and water treatment. This application is pursued in a forthcoming publication.

LITERATURE SURVEY

Most of the models which have been proposed concerning the void space of porous materials aim either at the study of the permeability of these materials or the determination of effective diffusion coefficients (for example, inside catalyst pellets). The present model belongs to the former class and is concerned with the void space among the grains of packed beds rather than the micropore structure which individual grains, such as active carbon granules, may possess. A critical review of the earlier of models concerned with the permeability of porous structures has been presented by Scheidegger (1961). Scheidegger has classified these into capillaric models, hydraulic radius theories, drag theories of permeability, and statistical theories. One should, perhaps, distinguish between statistical theories that treat bulk phenomena on an average basis while ignoring local structural details and statistical models which are concerned with local structural details and attempt to predict bulk phenomena based on an assumed pore structure of statistical nature. Thus, the present model would be classified as a statistical model.

The first statistical model was advanced by Childs and Collis-George (1950). These authors recognized that even if the porous structure could be considered as a bundle of capillary tubes, one could not casually assume that these tubes are of identical size. Instead, they have diameters with a certain random distribution—the pore size distribution. Such a distribution can be obtained, approximately, from saturation versus capillary pressure data. Based upon the calculation of the probability of occurrence of pairs of pores of all possible sizes together with some other assumptions, Childs and Collis-George obtained an expression for the permeability of isotropic porous media. Their expression, however, contains one parameter which has to be determined experimentally from pressure drop versus flow rate data. Although the expression does not provide a complete prediction of the permeability, it leads to a significantly better correlation of experimental data than that based on Kozeny's model. Subsequently, several statistical models were proposed which approximated the pore structure with networks of capillary tubes. The models advanced by Josselin de Jong (1958) and Saffman (1960) are based on random networks of uniform capillary tubes and were proposed for the prediction of dispersion coefficients. The model proposed by Fatt (1956) allows for the nonuniformity of the pores and aims at the prediction of the permeability and the relationship of saturation versus capillary pressure of isotropic media. An improved version of a random network of capillary tubes was advanced recently by Haring and Greenkorn (1970). This model has the attractive feature of considering randomly sized, randomly oriented pores. However, as it stands, it has a built-in inconsistency when it is applied to packed beds. From a simple geometrical consideration, it can be seen that the effective diameter of the smallest possible constriction in a packed bed of spheres is certainly larger than $(2\sqrt{3}/3 - 1)d_{g,\min} \simeq 0.155\ d_{g,\min}$, where $d_{g,\min}$ is the diameter of the smallest sphere of the bed. Any cylindrical pore of a model of a bed of this type should, therefore, have a diameter not smaller than $0.155\ d_{g,\min}$. This is not the case with their model, which assumes that there exist cylindrical pores with diameters less than this value. Since the reported calculated average pore diameter by Pakula and Greenkorn (1971) is, actually, slightly smaller than $0.155\ d_{g,\min}$, the above argument is not a minor objection. A direct consequence of this inconsistency seems to be that the calculated average pore length is only about half the average grain diameter, while it should be about equal.

Models which involve use of capillary cylindrical tubes are inadequate for the modeling of filtration through packed beds, since they do not account for the curvature of the surface of the grains, which, in this case, is of primary importance. Furthermore, such models, by neglecting the converging-diverging character of the flow, cannot account for the establishment of inertia effects in packed beds at values of the Reynolds number which are at least two orders of magnitude lower than the critical Reynolds number value in a smooth cylindrical tube. Clearly, for the study of these phenomena in packed beds, a model which retains the converging-diverging character of the flow is called for. The work by Snyder and Stewart (1966) pertaining to regularly packed beds of uniform spheres, is an important contribution in this area, but unfortunately it has not been extended to the case when the inertia terms are not negligible, and also it is not directly applicable to randomly packed beds.

FORMULATION OF THE MODEL

Description of the Model

For purposes of clarity, the definitions of certain terms to be used in describing the model will be stated first. The large cavities occupying the spaces among the grains of the packed bed will be referred to as pores; these cavities are often referred to as caverns. A packed bed can be considered to be an array of pores, each of which is connected with its neighboring pores through narrow channels which are called constrictions. The walls of these constrictions do not possess axial symmetry, but, for simplicity, it is assumed that they do. Accordingly, each constriction can be characterized by the diameter of its most narrow cross section. Let the minimum diameter of such a constriction be denoted by d_c; d_c is clearly a random variable and its probability distribution function will be referred to as the constriction size distribution CSD. It will also be assumed that each pore can be characterized by a single characteristic length, the effective pore diameter denoted by d_p. The pore diameter is also a random variable with a certain distribution, which will be referred to as the pore size distribution PSD. The latter term has a different meaning here from what is conventionally understood. In the main body of literature dealing with capillaric models the term pore size distribution is synonymous with the distribution of the diameters of the conceptual capillary tubes. To avoid confusion, we will refer to distributions of the latter type as capillary pore size distributions CPSD.

The model is formulated on the following basis. Let l be the length defined so that a cubic volume element of the bed with side equal to Nl contains a number of grains which tends to N^3 as N becomes very large. l is called the length of periodicity and is of the order of magnitude of the effective diameter of a grain of average volume. Consider a partition of the packed bed in layers of thickness l. These layers are statistically identical with each other. Therefore, one can study the entire bed in terms of a single layer of thickness l. A layer of packed bed of thickness l represents a unit bed element UBE. The determination of l, as well as the determination of other pertinent quantities, will be given in the next section.

Since the main flow in a packed bed is, generally, in the axial direction, the flow from any pore to neighboring ones at the same elevation (assuming that the flow direction is vertical) is expected to be relatively unimportant.* Accordingly, the existence of all constrictions connecting pores at the same elevation will be ignored. We will limit our consideration to constrictions connecting pores at different elevations. Since for a randomly packed bed the size of a constriction is independent of its orientation, it follows

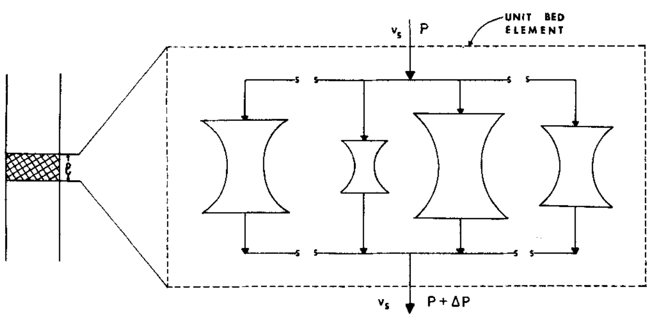

Fig. 1. Schematic representation of a unit bed element.

* This statement, of course, is incorrect if the main interest is to study the radial dispersion.

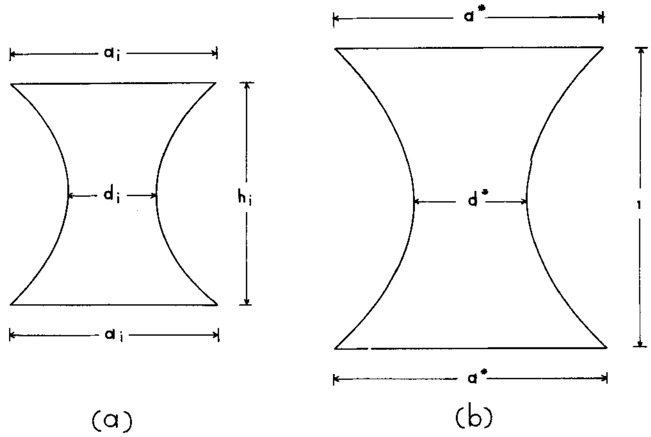

Fig. 2. (a). Dimensional unit cell of the *i*th type; (b). Dimensionless unit cell (same for unit cells of all types).

that the effective diameters of constrictions connecting pores at different elevations obey the same distribution as the effective diameters of the entire constriction population. Let N_c be the number of constrictions per unit area of any cross section of the bed. It will be assumed that all constrictions within a UBE lie on the middle plane (see Figure 1), and each constriction connects two half-pores. A pair of half-pores connected through a constriction constitutes a unit cell UC. There are N_c unit cells per unit area of UBE. Each UC resembles a piece of constricted tube.† The unit cells are not, in general, equal to each other. It will be assumed that there are exactly I_c different types of unit cells. Let n_i be the number fraction of unit cells of the ith type. It follows that there are n_iN_c unit cells of the ith type per unit area of UBE. Consider a single unit cell of the ith type, as shown in Figure 2a. Each cell has, by assumption, axial symmetry. It is also assumed that the plane perpendicular to the axis at the center of the unit cell is a plane of symmetry. The wall is assumed to be a parabola of revolution. The geometry of each cell is, therefore, uniquely determined by three dimensions, namely the constriction diameter d_i, the maximum diameter a_i, and the height h_i. The height of a unit cell should be about equal to the length of a curve which connects the centers of the two pores considered, passes through the center of the connecting constriction, and remains as far as possible from the wall at all elevations. Since in real beds a pore does not usually lie directly above or below one of its neighbors the length of this curve is somewhat greater, or at least equal, to the elevation difference between the centers of the two pores. Therefore, h_i is not necessarily less than or equal to the length of periodicity l. For some of the unit cell types it will be $h_i \leq l$ and for some $h_i > l$.

The following major assumptions will be made:

$$a_i = c_1 d_i \qquad i = 1, \ldots, I_c \tag{1}$$

and

$$h_i = c_2 d_i \qquad i = 1, \ldots, I_c \tag{2}$$

where c_1 and c_2 are constants to be determined. These assumptions have been based on the following reasoning. In a bed of randomly packed grains, on the average, large constrictions are formed among grains which are large and/or loosely packed. It follows that pores adjacent to large constrictions should be expected to be also large.

† The idea of using constricted tubes for modeling of porous media is not a new one. Petersen (1958) and Houpeurt (1959) have already coined this idea although they did not offer a method for the determination of the geometry of these tubes or the solution of the flow through them.

A similar argument leads to the inclusion that pores adjacent to small constrictions should be expected to be small.

Undoubtedly, assumptions besides those expressed by Equations (1) and (2) can be made on equally plausible grounds. However, Equations (1) and (2), aside from their simplicity, possess a salutary feature. Although unit cells of different types are unequal, unit cells of different types are geometrically similar. As a result, unit cells of all I_c different types can be reduced to be identical on a dimensionless basis (Figure 2b).

Based on the above description of the model, it follows that the geometry of each UBE is completely known if l, $\{d_i, n_i; i = 1, \ldots, I_c\}$, c_1, c_2, and N_c are determined.

DETERMINATION OF l, $\{d_i n_i;\ i = 1, \ldots, I_c\}$, c_1, c_2 AND N_c

In order to determine the various pertinent quantities involved in the model, the following experimental information must be available: sieve analysis of the grains or equivalent information, macroscopic porosity of the bed, and saturation versus capillary pressure data, particularly the initial drainage curve.

Determination of l

The length of periodicity can be determined from the requirement that a cube of side l contains, on the average, one grain of average volume; therefore,

$$(1-\epsilon)l^3 = \sum_{j=1}^{I_g} \nu_j (V_g)_j = \sum_{j=1}^{I_g} c_0 \nu_j (d_g)_j^3$$

or

$$l = \left[\frac{c_0}{(1-\epsilon)} <d_g^3> \right]^{1/3} \tag{3}$$

where I_g is the number of different sizes of grains of the packed bed, ν_j is the number fraction of grains with effective diameter $(d_g)_j$, $(V_g)_j$ is the volume of a grain with effective diameter $(d_g)_j$, and c_0 is a constant which arises from the assumption that

$$\frac{(V_g)_j}{(d_g)_j^3} = c_0 \qquad j = 1, \ldots, I_g \tag{4}$$

Assuming spherical grains, Equation (3) takes the form

$$l = \left[\frac{\pi}{6(1-\epsilon)} <d_g^3> \right]^{1/3} \tag{5}$$

Determination of the CSD, that is, $\{d_i, n_i; i = 1, \ldots, I_c\}$

The constriction size distribution is to be determined from the saturation versus capillary pressure curve which has been used to obtain capillary pore size distributions by previous investigators (Childs and Collis-George, 1950; and for extensive reviews of subsequent work, Dullien and Batra, 1970; Morrow, 1970). Several experimental procedures can be used to obtain saturation versus capillary pressure data. The one adopted in this work was developed by Haines (1930) and is well suited for packed beds of grains with size less than 1 mm. The principle on which this method is based is as follows: if a certain suction is applied on the water phase in a layer of a porous medium initially saturated with water and having one surface open to the air, the interface between water and air recedes to a certain extent into the porous layer. The phenomenon of water withdrawal from pores has been described by Childs (1969) and by Morrow (1970). The suction required to empty a pore depends on the size and shape of the largest of its constrictions at which the water-air interface exists.

The volume collected under a certain suction is related to the number of pores which are accessible through constrictions of size greater than a certain value. Hence, it is possible to quantify the number of constrictions of a given size. Some of the previous investigations have used the saturation-capillary pressure data for the estimation of CPSD's. In doing so, an assumption relating the diameter of the conceptual cylindrical pore to the size of the largest constriction of the corresponding real (noncylindrical) pore is required. This has been recognized by Childs (1969). The assumption that is commonly made is that the diameter of each cylindrical pore of the model is proportional to the effective diameter of the largest constriction of the corresponding real pore. In the present work the concept of cylindrical pores is not used. Instead, the initial drainage curve is used to determine the CSD.

Consider a typical initial drainage curve where the abscissa is $p_s^{-1} = (\rho g h_s)^{-1}$ and the ordinate is the saturation S. Let $\{S_{i-1/2};\ i = 1, \ldots, I_c, I_c + 1\}$ be a partition of the region $[S_{wi}, 1]$, and let $\{p_{i-1/2}^{-1};\ i = 1, \ldots, I_c, I_c + 1\}$ be the corresponding values of p_s^{-1}. I_c is the number of different constriction diameters to be considered and can be chosen arbitrarily as long as the value chosen is large enough for the required accuracy.

The effective diameter of a constriction corresponding to a certain suction p_s is obtained from

$$d_c = \frac{4\gamma_{12}\cos\theta_c}{p_s} \tag{6}$$

where γ_{12} is the water-air surface tension, and θ_c is the contact angle. The contact angle for a wetting withdrawing fluid is zero; it is not zero for an advancing fluid, even a wetting one. This can be deduced from the results of Rose and Heins (1962). They found that while a receding angle of a wetting fluid is zero (or near-zero), advancing angles depend on the rate of advancement and increase with the increase of the interface velocity. Since the value of θ_c is less ambiguous during drainage, the use of the initial drainage curve for the calculation of CSD's is preferred. Imbibition curves should not be used in view of the ambiguity of the value of the contact angle during advancement. The secondary or subsequent drainage curves should not be used also if they do not coincide with the initial curve. Such discrepancies would indicate the entrapment of air bubbles in the pores of the sample during the first imbibition. For the initial drainage curve, $\theta_c \cong 0$, and Equation (6) becomes

$$d_c \cong \frac{4\gamma_{12}}{p_s} \tag{7}$$

Let

$$d_i = \frac{1}{2}(d_{i-1/2} + d_{i+1/2}) \cong 2\gamma_{12}\left(\frac{1}{p_{i-1/2}} + \frac{1}{p_{i+1/2}}\right) \qquad i = 1, \ldots, I_c \tag{8}$$

It remains to determine the number fraction of constrictions with effective diameter between $d_{i-1/2}$ and $d_{i+1/2}$, that is, approximately equal to d_i for $i = 1, \ldots, I_c$.

In order to accomplish this, certain assumptions will be made. Let the effective volume of a pore V_{pe} be defined as the total volume of the pore minus the volume of those parts of the pore which remain occupied by pendular water at atmospheric pressure and the temperature of the experiment. These parts are occupied by virtually stagnant liquid even at high flow rates through the main pore volume. It will be assumed that the effective diameter of a pore is related to its effective volume in the same way as the effective grain diameter to the volume of the grain.* This assumption together with the assumption expressed by Equation (4) gives

$$\frac{(V_{pe})_i}{(d_p)_i^3} = \frac{(V_g)_j}{(d_g)_j^3} = c_0 \quad i = 1, \ldots, I_p; \; j = 1, \ldots, I_g \tag{9}$$

As mentioned earlier d_p is a random variable. The pore size distribution PSD, however, is not known. It is conceivable that for certain types of porous media, such as porous rocks, catalyst pellets, etc., there is no correlation between the effective diameter of a pore and the effective diameter of its largest constriction. However, for randomly packed beds of monosized, or nearly monosized, grains one would expect that these two random variables are related in some manner. It will be assumed that

$$(d_p)_i = c_3 d_i \quad i = 1, \ldots, I_c; \; I_p = I_c \tag{10}$$

where c_3 is a constant. The justification for this assumption is the same as that used in connection with Equations (1) and (2). Then, one has

$$V_t(S_{i+1/2} - S_{i-1/2}) = (\Delta N_i)(V_{pe})_i = (\Delta N_i)\, c_0\, (d_p)_i^3 \tag{11}$$

where ΔN_i is the total number of pores the largest constrictions of which have values within the interval $[d_{i-1/2}, d_{i+1/2}]$. The left-hand side of Equation (11) represents the volume of liquid collected experimentally when the suction pressure is increased from $p_{i+1/2}$ to $p_{i-1/2}$, while the right-hand side represents the total effective volume of pores from which this amount of liquid is withdrawn. Using Equation (11) and invoking the assumption expressed by Equation (10), one obtains

$$n_i(d_i) \equiv \frac{\Delta N_i}{\sum_{i=1}^{I_c} \Delta N_i} = \frac{(S_{i+1/2} - S_{i-1/2})}{d_i^3} \left[\sum_{i=1}^{I_c} \frac{(S_{i+1/2} - S_{i-1/2})}{d_i^3} \right]^{-1} \quad i = 1, \ldots, I_c \tag{12}$$

where $n_i(d_i)$ is the number fraction of pores each of which has at least one constriction with effective diameter from the interval $[d_{i-1/2}, d_{i+1/2}]$, or approximately equal to d_i, and the rest constrictions with diameters less than d_i. It will be assumed that $n_i(d_i)$ is also the number fraction of constrictions with effective diameters equal to d_i. This assumption is a fairly reasonable one, but one should be aware of the fact that it is only roughly valid and that it is more biased in the region of small diameter values, since smaller constrictions are, in general, more likely to escape detection during the saturation versus capillary pressure experiment than are large constrictions. This nonuniform bias is due to the fact that if a water-air interface exists at a number of constrictions of a pore, it is always the interface at the largest of these constrictions that gives in first under increasing suction values. However, this bias is cancelled, to a certain extent, from the presence of pores which would regularly be emptied under a certain suction value, but which are surrounded exclusively by pores that can only be emptied at considerably higher suctions. When one of the latter pores is finally emptied, the pore with large constrictions connected to it is also been emptied at that time, resulting in an inflation of the measurement corresponding to the smaller constriction being investigated at the time.

Equation (12), subject to the postulated assumptions, provides a means of estimating the CSD from the initial drainage curve.

Determination of c_1 and c_2

For the determination of the dimensions of a unit cell, it is assumed that

$$a_i = (d_p)_i \quad i = 1, \ldots, I_p; \; I_p = I_c \tag{13}$$

that is, the maximum diameter of a unit cell is equal to the effective diameter of the pores involved [based on Equation (10) the two half-pores comprising a unit cell belong to pores of equal effective diameters]. Equations (1), (10), and (13) give $c_1 = c_3$ and, therefore,

$$a_i = (d_p)_i = c_1 d_i = c_3 d_i \quad i = 1, \ldots, I_c \tag{14}$$

In order to determine values for the constants c_1 and c_2 the following constraints are imposed:

$$\epsilon(1 - S_{wi})l^3 = \sum_{i=1}^{I_c} n_i (V_{pe})_i \tag{15}$$

and

$$<h> \equiv \sum_{i=1}^{I_c} n_i h_i = \sum_{j=1}^{I_g} \nu_j (d_g)_j \equiv <d_g> \tag{16}$$

Equation (15) is a simple effective void volume balance. The constraint expressed by Equation (16) requires some elaboration. As was mentioned earlier, h_i is allowed to be larger than, equal to, or smaller than l. On the average, one expects h_i to be approximately equal to the diameter of the grains which form the wall of the unit cell. Since both the grain diameter and the height of the unit cell are random variables, the constraint is expressed in terms of the respective means. c_1 can be obtained by combining Equations (3), (9), (14), and (15):

$$c_1 = \left[\frac{\epsilon(1 - S_{wi})}{(1 - \epsilon)} \frac{<d_g^3>}{<d_c^3>} \right]^{1/3} \tag{17}$$

Equations (2) and (16) give

$$c_2 = \frac{<d_g>}{<d_c>} \tag{18}$$

Equations (1) and (17) give

$$a_i = \left[\frac{\epsilon(1 - S_{wi})}{(1 - \epsilon)} \frac{<d_g^3>}{<d_c^3>} \right]^{1/3} d_i \quad i = 1, \ldots, I_c \tag{19}$$

Equations (2) and (18) give

$$h_i = \frac{<d_g>}{<d_c>} d_i \quad i = 1, \ldots, I_c \tag{20}$$

Determination of N_c

The determination of the number of constrictions per unit cross section of the bed is made as follows. Consider an array of randomly packed spheres the diameters of which have a certain frequency distribution function. Consider further a plane cutting through this array. The orientation of this plane is of no consequence due to the assumption of complete randomness of packing. This plane cuts through a number of spheres, which results in the formation of a number of circles on the plane. Wicksell (1925) determined theoretically the frequency distribution

* This assumption is akin to Rumpf's conception of a packed bed as a mixture of solid and void grains (mentioned by Debbas and Rumpf, 1966).

function of the diameters of the circles in terms of the frequency distribution function of the diameters of the randomly packed spheres. His results can be utilized to determine N_c, if, for this purpose, one assumes that the pores of randomly packed beds of grains form a random array of spheres. Let $f_p(d_p)$ be the frequency distribution function of the diameters of the pores and $f_{pc}(d_{pc})$ the frequency distribution function of the diameters of the circles on any section plane. Wicksell's result can be written as

$$f_{pc}(d_{pc}) = \frac{d_{pc}}{<d_p>} \int_{d_{pc}}^{(d_p)_{max}} f_p(x)\,(x^2 - d_{pc}^2)^{-1/2}\,dx \tag{21}$$

Consider a plane cutting through the array of pores which is normal to the axis of the packed bed. Assuming that each circle appearing on this plane corresponds to a unit cell, in other words, assuming that the number of circles per unit area of plane is equal to N_c, it follows from a void volume balance that

$$N_c \int_0^{(d_p)_{max}} \frac{\pi}{4} y^2 f_{pc}(y)\,dy = \epsilon(1 - S_{wi}) \tag{22}$$

Substituting f_{pc} from Equation (21) into Equation (22), one obtains

$$N_c = \frac{4\epsilon(1 - S_{wi}) <d_p>}{\pi \int_0^{(d_p)_{max}} \int_y^{(d_p)_{max}} y^3 f_p(x)\,(x^2 - y^2)^{-1/2}\,dx\,dy} = \frac{6\epsilon(1 - S_{wi}) <d_p>}{\pi <d_p^3>} \tag{23}$$

Equation (23) was obtained for a continuous frequency distribution function for the effective pore diameter. It is obvious that the same result also holds for discrete distributions. Equation (23) relates N_c to the pore size distribution. Using Equations (14) and (17), N_c can be further related to the constriction size distribution as shown in the following section.

Summary of Relations—Dimensionless Unit Cell

It is expedient to consider the unit cells in dimensionless form. The following dimensionless quantities are introduced:

$$a_i^* = \frac{a_i}{h_i},\ d_i^* = \frac{d_i}{h_i},\ h_i^* = \frac{h_i}{h_i} \quad i = 1, \ldots, I_c \tag{24}$$

Using Equations (14), (19), (20), (23), and (24), one obtains

$$h_i^* = 1 \quad i = 1, \ldots, I_c \tag{25}$$

$$d_i^* = \frac{<d_c>}{<d_g>} \equiv d^* = \text{const.} \quad i = 1, \ldots, I_c \tag{26}$$

$$a_i^* = \frac{<d_c>}{<d_g>} \left[\frac{\epsilon(1 - S_{wi})}{(1 - \epsilon)} \frac{<d_g^3>}{<d_c^3>} \right]^{1/3} \equiv a^* = \text{const.} \quad i = 1, \ldots, I_c \tag{27}$$

$$N_c = \frac{6\epsilon(1 - S_{wi}) <d_c>}{\pi <d_c^3>} \left[\frac{(1 - \epsilon)}{\epsilon(1 - S_{wi})} \frac{<d_c^3>}{<d_g^3>} \right]^{2/3} \quad i = 1, \ldots, I_c \tag{28}$$

with h_i given by Equation (20), l given by Equation (5) and the means $<d_c>$ and $<d_c^3>$ based on the CSD given by Equation (12). It is worth noting that in dimensionless form all unit cells of a given granular randomly packed bed are, according to the postulated model, identical. This feature is particularly attractive in view of the fact that the solution of the flow problem through each unit cell can only be carried out with numerical methods.

APPLICATION OF THE MODEL: FLOW THROUGH PACKED BEDS

The ultimate objective of this work is the formulation of a model of granular randomly packed beds suitable for the description of deep bed filtration. Before this can be accomplished, the flow information through the bed based on the postulated model needs to be obtained. Furthermore, as a first step in model validation, the calculated flow data should be in good agreement with experimental results.

In accordance with the proposed model, the pressure drop along the various unit cells in a given unit bed element should be the same. The flow rates of different unit cells will, of course, be different and the total flow rate through all the N_c cells in a unit cross section is numerically equal to the superficial velocity. The flow through an individual unit cell is governed by the Navier-Stokes equation, appropriately simplified. The solution is obtained under the assumption of two dimensional, steady state, incompressible flow. The inertia terms are not neglected. Since the partial differential equation is of the elliptic type, boundary conditions at the inlet and outlet of the unit cell need to be specified. For this reason, it is assumed that each unit cell is attached to two tubes both of which are semi-infinite in length and are formed by the repetition of the cell under consideration. All the dimensional unit cells are reduced to a single dimensionless periodically constricted tube, Figure 3, and the flow problem to be solved is the steady state, fully developed flow through this tube, at various Reynolds numbers. The mathematical formulation of the problem and the numerical algorithm which was developed for its solution are given in a companion paper (Payatakes, Tien, and Turian, 1972).

Let ΔP be the common pressure drop along each unit cell of a given unit bed element. The pressure gradient along the packed bed, according to the postulated model,

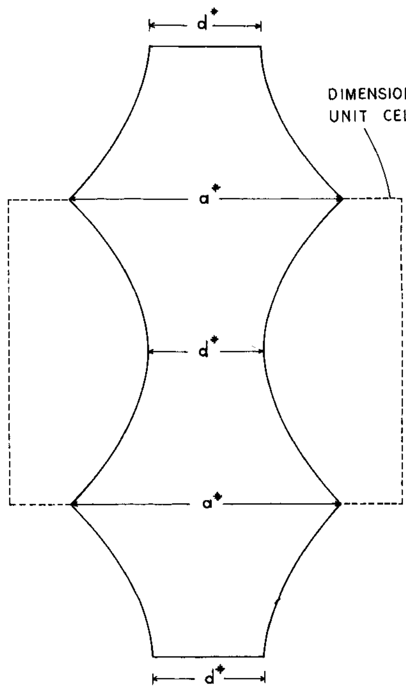

Fig. 3. Extended dimensionless unit cell (same for unit cells of all types).

is $\Delta P/l$. The friction factor of packed beds is defined by

$$f_s = -\frac{<d_g> \Delta P}{2\rho l v_s^2} \quad (29)$$

and the superficial Reynolds number by

$$(N_{Re})_s = \frac{<d_g> v_s}{\nu} \quad (30)$$

We seek the relationship which gives f_s as a function of $(N_{Re})_s$. For a given ΔP, let q_i be the flow rate through each unit cell of the ith type. $q_i \neq q_j$ for $i \neq j$. Let

$$(v_0)_i = \frac{4q_i}{\pi d_i^2} \quad i = 1, \ldots, I_c \quad (31)$$

and

$$(N_{Re})_i = \frac{h_i(v_0)_i}{\nu} \quad i = 1, \ldots, I_c \quad (32)$$

where $(v_0)_i$ is the characteristic velocity, and $(N_{Re})_i$ the Reynolds number for each unit cell of the ith type. Let

$$\Delta P_i^* = \frac{\Delta P}{\rho (v_0)_i^2} \quad i = 1, \ldots, I_c \quad (33)$$

be the dimensionless pressure drop along a unit cell of the ith type. Although all unit cells reduce to the same dimensionless unit cell, and the pressure drop ΔP is the same for all cells, the dimensionless pressure drop along cells of different types is different. The solution of the problem of flow through the dimensionless unit cell depends on the geometry of the cell and on the Reynolds number. For laminar flow one can obtain (see Payatakes, Tien and Turian, 1972) the dimensionless pressure drop as a function of the Reynolds number and the geometry,

$$\Delta P_i^* = \phi_0 [(N_{Re})_i; a^*, d^*] \quad i = 1, \ldots, I_c \quad (34)$$

Once relation (34) is available, one can calculate the friction factor as a function of $(N_{Re})_s$ even for high values of $(N_{Re})_s$, where the inertia terms are appreciable, using interpolation.

If the Reynolds number is sufficiently low, Equation (34) has the simple form

$$\Delta P_i^* = \phi_0 [(N_{Re})_i; a^*, d^*] = \frac{\phi_0(1; a^*, d^*)}{(N_{Re})_i} = \frac{\Delta P_1^*}{(N_{Re})_i} \quad (35)$$

where

$$\Delta P_1^* \equiv \phi_0(1; a^*, d^*) \quad (36)$$

In this case, f_s is given by

$$f_s = -\left[\frac{2 <d_c> <d_g>}{N_c \pi l <d_c^3>}\right] \frac{\Delta P_1^*}{(N_{Re})_s} \quad (37)$$

In the above expression l is given by Equation (5), d^* is given by Equation (26), a^* is given by Equation (27), N_c is given by Equation (28), and $<d_c>$ and $<d_c^3>$ should be calculated based on the CSD as given by Equation (12). Equation (37) gives the friction factor of a packed bed as a function of $(N_{Re})_s$ and two factors, one of which is completely determined from geometric characteristics of the bed. The other ΔP_1^* is the dimensionless pressure drop per unit dimensionless length along a periodically constricted tube which is formed by the repetition of a dimensionless unit cell with height equal to unity, constriction diameter d^*, maximum diameter a^*, and wall which is a parabola of revolution, at $N_{Re} = 1$. This quantity can be calculated numerically. This calculation has been carried out for several representative values of a^*

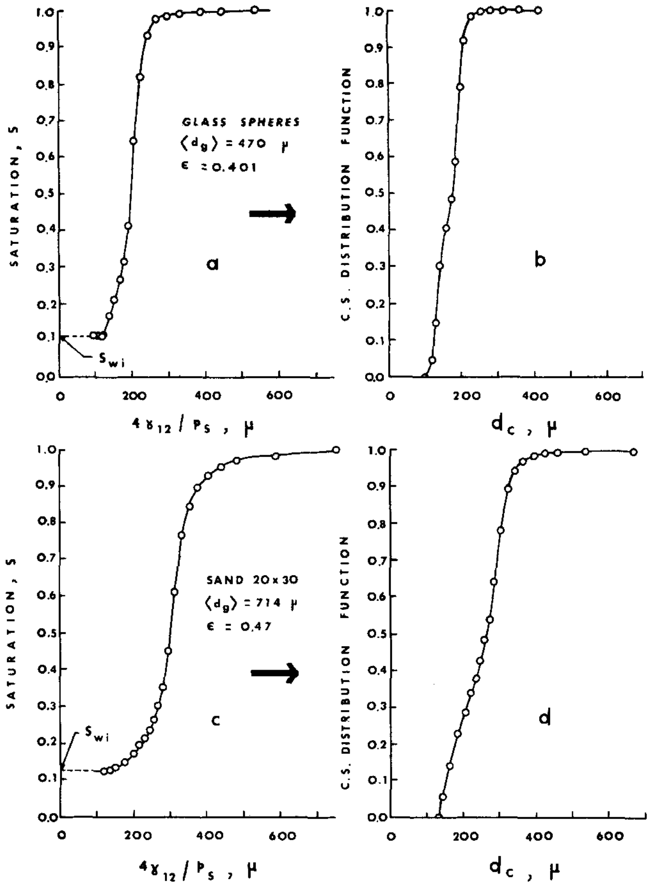

Fig. 4. Saturation-capillary pressure data and corresponding calculated constriction size distributions.

and d^* in the range $0.733 \leq a^* \leq 1$ and $0.250 \leq d^* \leq 0.600$ using $\kappa^* = 1/36$. This range should suffice for most packed beds composed of grains which are used in practice.

These results have been interpolated in order to obtain the following approximate analytical expression for ΔP_1^*:

$$-\Delta P_1^* = A_0(a^*) + A_1(a^*) d^* + A_2(a^*) d^{*2} + A_3(a^*) d^{*3} \quad (38)$$

where

$$A_0(a^*) = 502.669 - 108.497a^* - 57.730a^{*2} \quad (39)$$

$$A_1(a^*) = -914.276 - 1670.718a^* + 1391.069a^{*2} \quad (40)$$

$$A_2(a^*) = 260.109 + 5328.505a^* - 3772.042a^{*2} \quad (41)$$

$$A_3(a^*) = 599.147 - 4749.109a^* + 3130.690a^{*2} \quad (42)$$

In the region of validity of Equation (37), that is, as long as the inertia terms of the Navier-Stokes equation are negligibly small, the flow rate through a unit cell of the ith type for a given value of v_s is given by

$$q_i = \frac{v_s d_i^3}{N_c <d_c^3>} \quad i = 1, \ldots, I_c \quad (43)$$

COMPARISON WITH EXPERIMENTAL RESULTS

The modeling method developed in the preceding sections is applied here to two different randomly packed beds and compared with the corresponding experimental data. One is composed of glass beads with nominal diameter of 470μ and has porosity of 0.401. The other is composed of sand 20 $\times$ 30 grains and has porosity of 0.47. Saturation versus capillary pressure data were obtained for both beds. These data together with the calculated CSD's are given in Figure 4. Based on this information one can obtain the values summarized in Table 1. The experimental and the calculated relationship between f_s and $(N_{Re})_s$ are given in Figure 5 for the bed of glass spheres and in Figure 6 for the bed of sand. As can be seen, the model developed in this work gives a correct prediction of the effect of the inertia terms on the friction factor. This effect is detectable even at $(N_{Re})_s < 5$ and increases rapidly with $(N_{Re})_s$. The calculated friction factor values are within +12% in the case of the bed of sand and −4% in the case of the bed of glass spheres.

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NOTATION

A_c = cross section area of the bed
$A_0(a^*)$, $A_1(a^*)$, $A_2(a^*)$, $A_3(a^*)$ = interpolating polynomials
a_i = maximum diameter of a unit cell of the ith type
a^* = maximum diameter of the dimensionless unit cell
a_i^* = dimensionless maximum diameter of a unit cell of the ith type
c_0, c_1, c_2, c_3 = constants related to the geometry of the porous medium

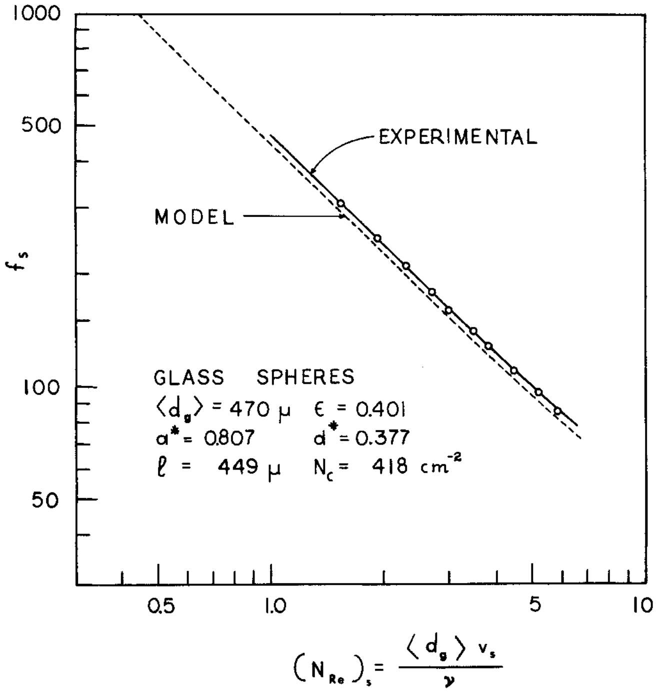

Fig. 5. Experimental and theoretical relation between friction factor and superficial Reynolds number for a bed of spheres.

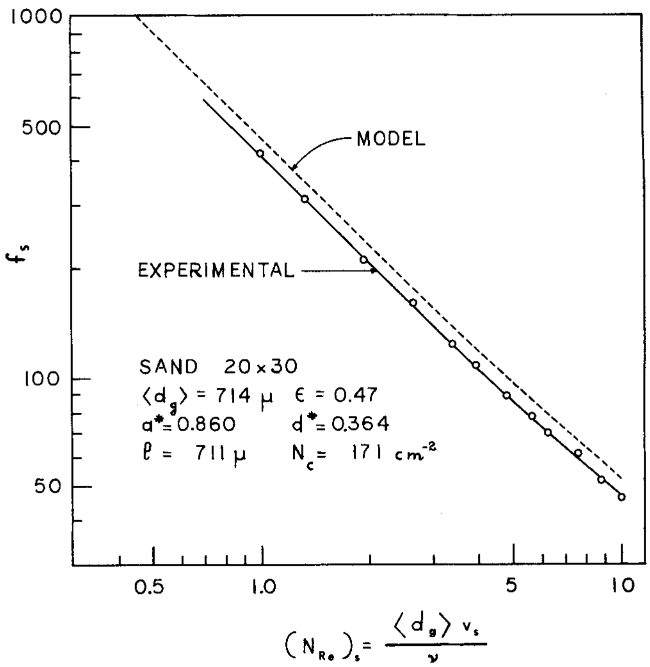

Fig. 6. Experimental and theoretical relation between friction factor and superficial Reynolds number for a bed of sand grains.

TABLE 1. APPLICATION OF THE MODEL

Quantity	Glass Beads	Sand
ϵ	0.401	0.47
$<d_g>$, cm	0.0470	0.0714
$<d_g^3>$, cm^3	0.1038×10^{-3}	0.3640×10^{-3}
S_{wi}	0.111	0.127
$<d_c>$, cm	0.0177	0.0260
$<d_c^3>$, cm^3	6.272×10^{-6}	21.429×10^{-6}
c_1	2.141	2.363
c_2	2.652	2.747
h^*	1.0	1.0
a^*	0.807	0.860
d^*	0.377	0.364
l, cm	0.0449	0.0711
N_c, cm^{-2}	418.0	171.0
ΔP_1^* [Eq. (38)]	−101.06	−100.94
$\Delta P_1^* \left[\text{direct calc.; } \kappa^* = \frac{1}{36} \right]$	−100.7	−101.1
$f_s \cdot (N_{Re})_s$ for $(N_{Re})_s < 5$	454.0	460.0

d_c = effective constriction diameter
d_g = effective grain diameter
$\{(d_g)_j;\ j = 1, \ldots, I_g\}$ = set of different effective diameters of grains present in the bed
$d_{g,\min}$ = diameter of the smallest sphere in a bed of spheres
d_i = constriction diameter of a unit cell of the ith type
$\{d_{i-1/2};\ i = 1, \ldots, I_c + 1\}$ = constriction diameters corresponding to the set of suction values $\{p_{i-1/2};\ i = 1, \ldots, I_c + 1\}$
d_p = effective pore diameter
$\{(d_p)_i;\ i = 1, \ldots, I_p\}$ = set of different effective diameters of pores present in the bed
$(d_p)_{\max}$ = maximum value of d_p
d^* = constriction diameter of the dimensionless unit cell
d_i^* = dimensionless constriction diameter of a cell of the ith type
$f_p(d_p)$ = frequency distribution function of the effective pore diameter
$f_{pc}(d_{pc})$ = frequency distribution function of the diameters of the circular traces on a plane cutting through a random array of spheres
f_s = friction factor of a packed bed
g = constant of gravitational acceleration
h_i = height of a unit cell of the ith type
h_s = elevation difference between the free water surface and the packed layer in the saturation versus capillary pressure experiment
h_i^* = dimensionless height of a unit cell of the ith type
I_c = number of different types of unit cells
I_g = number of different sizes of grains composing the bed
I_p = number of different sizes of pores
i, j = indices
l = length of periodicity of the bed
N_c = number of constrictions per unit area of a bed cross section; also, number of unit cells per unit area of a unit bed element
$(N_{Re})_s$ = superficial Reynolds number
$(N_{Re})_i$ = Reynolds number characterizing the flow through a unit cell of the ith type
n_i = number fraction of pores, the largest constrictions of which have values within the interval $[d_{i-1/2}, d_{i+1/2}]$; also, by assumption, the number fraction of unit cells of the ith type
p_s = suction applied to the liquid phase in the saturation versus capillary pressure experiment
$\{p_{i-1/2};\ i = 1, \ldots, I_c + 1\}$ = set of arbitrarily chosen values of suction covering the entire region of interest of the initial drainage curve diagram
Q = flow rate through the bed
q_i = flow rate through a unit cell of the ith type
S = saturation
S_{wi} = irreducible saturation
$\{S_{i-1/2};\ i = 1, \ldots, I_c + 1\}$ = set of saturation values corresponding to the set of suction values $\{p_{i-1/2};\ i = 1, \ldots, I_c + 1\}$
$(V_g)_j$ = volume of a grain with effective diameter $(d_g)_j$
$(V_{pe})_j$ = effective volume of a pore with effective diameter $(d_p)_j$
V_t = total volume of liquid initially present in the sample in the saturation versus capillary pressure experiment
v_s = superficial velocity = Q/A_c
$(v_0)_i$ = characteristic velocity for a unit cell of the ith type

Greek Letters

γ_{12} = water-air surface tension
ΔN_i = total number of pores the largest constrictions of which have values within the interval $[d_{i-1/2}, d_{i+1/2}]$
ΔP = pressure drop along a unit cell for a given value of v_s
ΔP_i^* = dimensionless pressure drop along a unit cell of the ith type for a given value of v_s
ΔP_1^* = dimensionless pressure drop per segment of a periodically constricted tube with maximum diameter equal to a^*, minimum diameter equal to d^*, and walls which are parabolae of revolution, at $N_{Re} = 1$
ϵ = macroscopic porosity of the bed
θ_c = contact angle
κ^* = network increment used for the numerical solution of the flow
ν = kinematic viscosity
ν_j = number fraction of grains with effective diameter $(d_g)_j$
ρ = density of liquid
ϕ_0 = formal function

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Part II. Numerical Solution of Steady State Incompressible Newtonian Flow Through Periodically Constricted Tubes

A numerical method for the solution of the problem of steady state, incompressible Newtonian flow through periodically constricted tubes is developed. All terms of the Navier-Stokes equation are retained, including the nonlinear inertia terms.

Sample calculations for a uniform periodically constricted tube, the geometry of which is connected with the modeling of a packed bed of sand are given, including streamlines, axial and radial velocity profiles, pressure profiles, and the dimensionless pressure drop versus Reynolds number relation. The effect of some geometric characteristics of periodically constricted tubes on their friction factor is investigated numerically, and comparison of some existing experimental data with calculated ones is made.

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SCOPE

The main purpose of this work is the development of a numerical method for the solution of the laminar steady state flow of an incompressible Newtonian fluid through a periodically constricted tube. This problem arises in the modeling of porous media. Petersen (1958) and Houpeurt (1959) have introduced capillaric models involving periodically constricted tubes. In Part I of this paper, the authors developed a statistical model for randomly packed beds of monosized or nearly monosized grains involving unit cells, each one of which resembles a segment of a periodically constricted tube, and they have proposed that the flow through any one of these unit cells can be identified with the flow through a segment of an infinitely long periodically constricted tube formed by the repetition of the unit cell under consideration. The detailed knowledge of the flow through the unit cells is necessary for the calculation of the permeability as well as for the modeling of any process which takes place in the void space of a packed bed, for example, the filtration of suspensions through packed beds encountered in water and waste water renovation and the filtration of feedstocks to catalytic beds in the oil industry. Beyond these specific applications, the solution of the problem will most probably be of use in future work in the modeling of porous media. The formulation of statistical models for anisotropic porous media involving constricted-tube type unit cells does not seem to be beyond reach, and the present work would be directly applicable to such models. Furthermore, application of the present work is not confined only to the case of periodically constricted tubes; the developed algorithm can be used to solve the problem through any tube of nonuniform cross section, such as venturi tubes, partially clogged arterial flows, tubes with step changes of diameter, and so on.

CONCLUSIONS AND SIGNIFICANCE

A numerical method was developed for the solution of the laminar steady state flow of an incompressible Newtonian fluid through both uniform and nonuniform periodically constricted tubes. The (nonlinear) inertia terms of the Navier-Stokes equation are retained. The solution is obtained in terms of the stream function and the nonvanishing component of the vorticity vector. Based on this information, the axial and radial components of the velocity vector as well as the pressure distribution are readily obtainable. In terms of the stream function and vorticity the algorithm is of second order everywhere, except in the immediate vicinity of the wall, where the special discretization procedure results in a scheme which is, in general, of first order. The stability of the algorithm can be assured by proper adjustment of two weighting factors involved in the scheme. Sample calculations are carried