10/5-1-97 (1)

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M997052749

In Situ Bioremediation: A Network Model of Diffusion and Flow in Granular Porous Media

S. K. Griffiths, R. H. Nilson, R. W. Bradshaw

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550
for the United States Department of Energy
under Contract DE-ACO4-94AL85000

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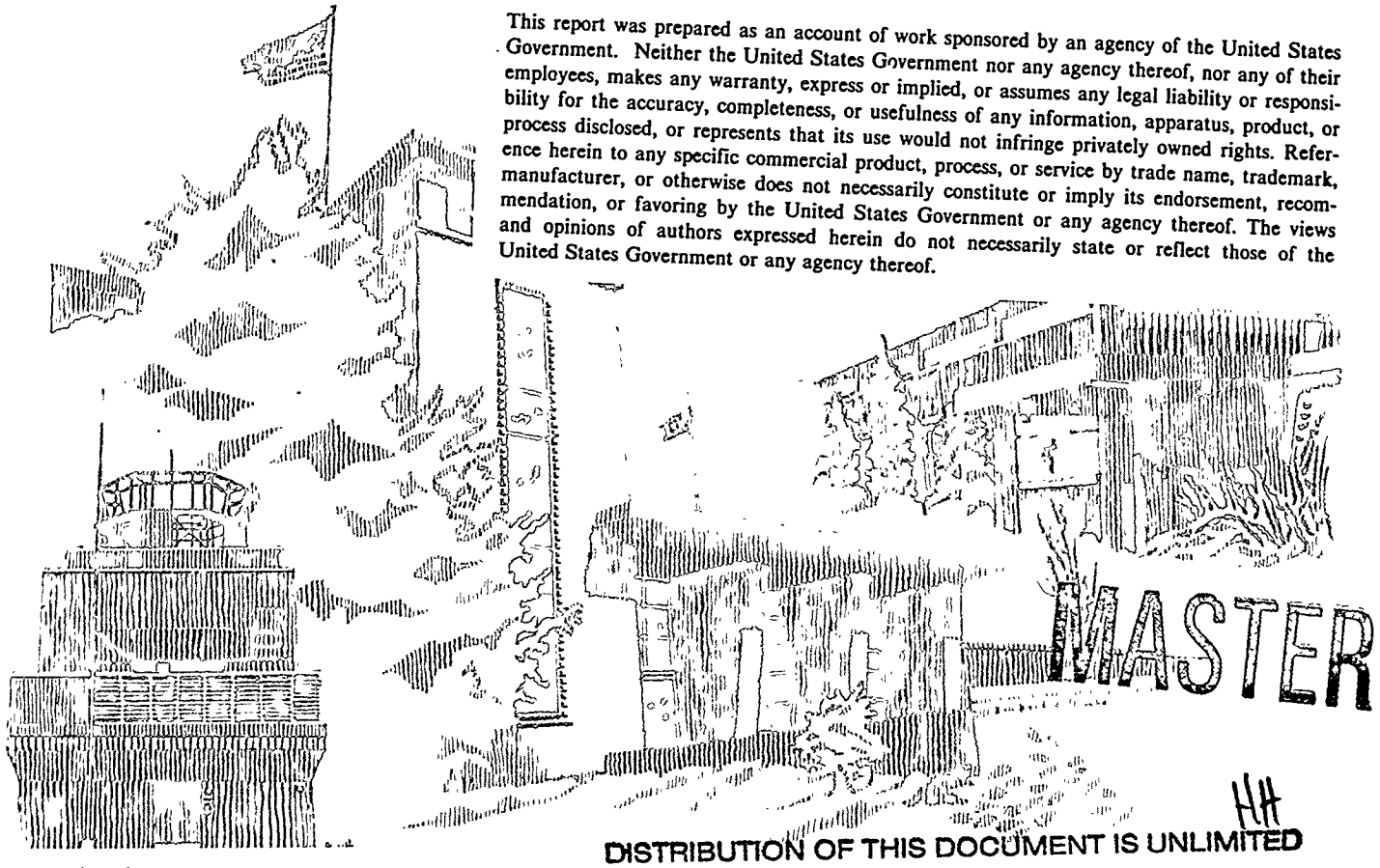

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IN SITU BIOREMEDIATION: A NETWORK MODEL OF DIFFUSION AND FLOW IN GRANULAR POROUS MEDIA

S. K. Griffiths, R. H. Nilson and R. W. Bradshaw
Sandia National Laboratories
Livermore, California 94551-0969

In situ bioremediation is a potentially expedient, permanent and cost-effective means of waste site decontamination. However, permeability reductions due to the transport and deposition of native fines or due to excessive microorganism populations may severely inhibit the injection of supplemental oxygen in the contamination zone. To help understand this phenomenon, we have developed a micro-mechanical network model of flow, diffusion and particle transport in granular porous materials. The model differs from most similar models in that the network is defined by particle positions in a numerically-generated particle array. The model is thus widely applicable to computing effective transport properties for both ordered and realistic random porous media. A laboratory-scale apparatus to measure permeability reductions has also been designed, built and tested.

INTRODUCTION

In situ bioremediation is a promising new technology for groundwater and soils decontamination, offering many potential benefits over both excavation and flushing [1,2,3]. Rather than extracting contaminants for subsequent treatment or permanent burial, this technique relies on microbial metabolisis to decompose contaminants in place, yielding biomass and harmless byproducts [4,5,]. Nearly all organic contaminants can be metabolized in this manner, including the recalcitrant pesticides, PCBs, and chlorinated dioxins, as well as the many common hydrocarbons [6,7,8].

Current estimates for the costs of waste site bioremediation range from $50-$80 per ton, as compared with $200 per ton or more for landfill disposal, and $250-$600 per ton for incineration [9]. Despite the apparent economic benefits, however, bioremediation is often not the preferred method for site restoration. The reason for this is in part because the technology is relatively new and in part because reliable predictive capabilities do not yet exist. Site managers cannot be assured a priori of the cost, duration and efficacy of bioremediation and so often opt for more direct though more costly alternatives. Improved understanding of bioremediation processes and improved capabilities for accurately predicting the duration and extent of cleanup would significantly increase the utility of this technology.

Successful application of bioremediation usually depends on injecting air, oxygen, oxygenated water or hydrogen peroxide to provide supplemental oxygen within the contamination zone [4,7]. Only in rare instances is bioremediation based on anaerobic decomposition [10,11]. Effective oxygenation of the contamination zone requires that soil permeabilities remain relatively high during the course of treatment. The treatment processes, however, may induce dramatic reductions in formation permeabilities. This phenomenon, known as formation blocking, usually results from one of three mechanisms: pore bubble nucleation due to the accumulation of gaseous decomposition products; pore plugging due to the long range transport and concentration of native fines; or pore plugging by the biomass resulting from excessive microorganism populations [12,13]. The two latter phenomena are the topic of our current study.

State-of-the-art modeling of bioremediation processes is generally based on three-dimensional, multicomponent, multiphase codes employing well established relative permeability transport algorithms [14,15]. These codes have been developed over nearly two decades to solve the somewhat simpler problem of subsurface contaminant transport [16]. The primary shortcoming of these codes in modeling bioremediation is that they neglect micro-scale phenomena in order to address the multidimensional macro-scale processes of the entire waste site [17,18]. Convective transport of particles and microorganisms is generally neglected, as is the effect of biomass on formation permeability. Similarly, most laboratory studies of biodegradation and bioremediation have concentrated on identifying specialized microorganisms and chemical environments which accelerate contaminant decomposition. While these studies consistently show the importance of supplemental oxygen to support the microorganism population, only a few have focused on the transport processes necessary to provide this oxygen in the contamination zone [12,14,19,20].

In the present study, we have developed a micro-mechanical network model intended to describe several micro-scale or sub-grid processes that are not explicitly treated in large-scale continuum models. A source listing of the program is given in Appendix A. One unique aspect of this model is its emphasis on particle transport and its effect on permeability. A primary goal of this work is to improve the

predictive capability of bioremediation modeling by helping to develop improved continuum correlations relating the macroscopic permeability and effective diffusivity to the evolved state of an interconnected pore structure. In addition, this research provides new capabilities for modeling fluid, species and particle motion in both ordered and random porous materials, with potential application to a wide range of micro-scale fluid transport and filtration problems.

In the experimental part of the present study, we have designed and built a laboratory-scale apparatus for measuring permeability reductions due to fines transport and deposition. Using this capability, we have made preliminary measurements of permeability reductions in glass spheres and in several common sands. The goal of this work was to provide permeability data on well characterized porous materials that would serve as a benchmark for the mathematical model.

NETWORK MODEL

Previous continuum models of plugging processes have failed to predict accurately the permeability reductions observed in laboratory and field experiments. This is true not only for bioremediation, but for more conventional filtration processes as well. Likewise, there has been very limited success with analytical models intended to describe plugging processes in terms of the reduction in throat size in a bundle of parallel capillary tubes. These classes of models fail to account for the interconnection among flow passages of differing sizes and the redistribution of flow that occurs as plugging proceeds.

To overcome these shortcomings we have developed a micro-mechanical network model that describes the internal structure of a random porous material as a system of interconnected tubes and nodes [21,22,23]. Tube networks such as these are generally constructed by placing tubes directly in the computational domain using a Poisson distribution or similar random process. Our approach differs from this in that the tube and node network is constructed about a collection of particles [24,25,26,27].

The computational domain is first symbolically packed with spherical particles from a specified size distribution. The size distribution is obtained by sampling spike, normal or log-normal distributions using a uniform random number generator. By this technique, a repeatable pseudo-random distribution of particle sizes of a specified mean and variance may be generated very quickly.

Once a particle size distribution is generated, the particles are assembled into a porous structure. To perform this task we have developed several packing algorithms. These appear in lines pages 3 through 19 of Appendix A. The first method employs a random number generator to place particles in a specified box, subject to

the constraint that no particles may inter-penetrate. This constraint may be further tightened to prevent the placement of a particle within a specified distance of any other. Particles are added in this manner to the box until a specified fractional density is obtained. This method is reasonably fast, but fractional densities greater than about 40% cannot be obtained by this technique. This is because granular materials having greater densities are not at all random.

To obtain high fractional densities, we have developed a second packing algorithm in which particles are added randomly to the top of the box. These particles are then moved downward (as though by gravity) until they arrive at the upper surface of those particles previously placed. When a falling particle first contacts another, the region around that fixed particle is examined numerically to determine the minimum energy state in which the new particle can be placed. The processes of adding individual particles is repeated until the box is full. This algorithm is quite slow since the size and location of many other particles must be checked as each new particle is packed. Despite the large effort required by this method, and the seemingly high degree of consolidation that should be obtained, fractional densities obtained by this method rarely exceed about 65%, depending on the size distribution of the particle set.

To obtain still high packing densities, we have developed a third algorithm in which all particles are initially placed by deterministic methods to obtain the desired density. Large particles are placed first in a regular packing. Smaller and still smaller particles are added later within the voids formed by those already placed. The resulting structure is highly ordered, and does not provide a good representation of a random material. To achieve greater disorder, each particle in the final set is sent on a random, noninterfering walk through the box. This is an extremely time consuming process, since the current position of each particle must be checked against all others in the box to ensure that inter-penetration does not occur. For the large computational price, however, fractional densities as high as the size distribution will permit may be obtained by this method.

Once the size and position of each particle has been determined, the network model is constructed. For this we have employed a subdivision of the space via a Voronoi tessellation [28]. This tessellation assigns each region of the domain to the closest particle. The Voronoi tessellation results in a polygon bounding each particle. The sides of these polygons form the skeleton of the network of channels surrounding the particles. A sample calculation showing the network at this stage is shown in Fig. 1. Note that each particle is bounded by several network channels. The most frequent number of bounding channels is five, though in large particle arrays as few as three and as many as twelve bounding channels may be seen. Also note that network channels always form intersections of three, and that these intersections define a unique node location at the end of each channel.

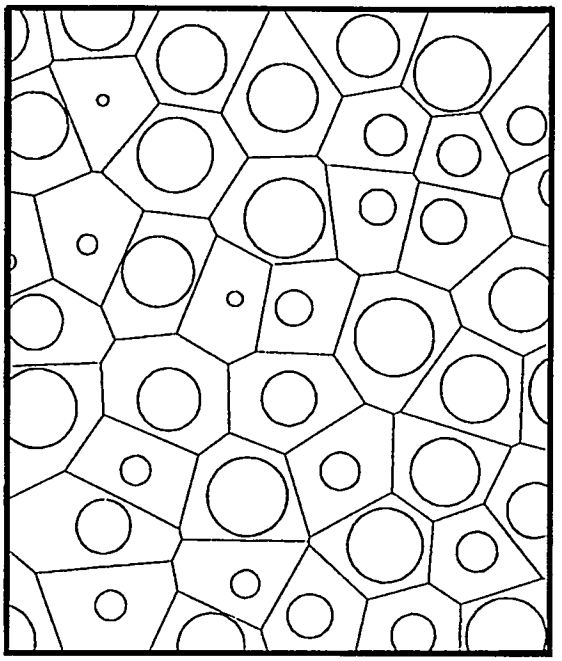


Figure 1. Schematic of particle array and corresponding Voronoi tessellation. The sides of the tessellation polygons form the network of channels through which fluid transport occurs.

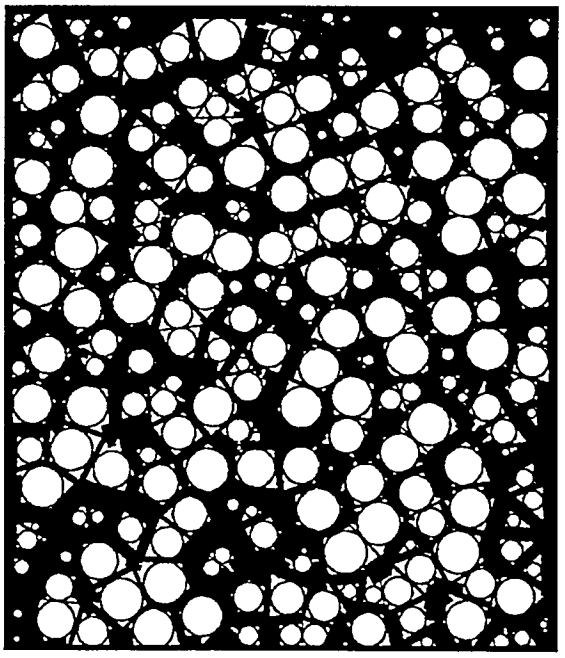


Figure 2. Schematic of particle array and channel network. Channel intersections define the nodes of the computational domain. Although these channels are displayed as having parallel walls, the governing transport equations take into account that channels conform to particle surfaces.

After the Voronoi tessellation is computed and the skeleton of the network is known, the nodes identified by pore tube intersections are numbered and cross correlated. This cross-correlation table provides a numerical map of connected node pairs and corresponding tube numbers, making the network a useful computational domain for solving the transport equations. Following construction of the network skeleton, channel sizes for each segment of the network are computed using the known center positions and radii of the two particles defining each channel segment. The source listing of the tessellation algorithm and method of network construction appears in pages 19 through 35 of Appendix A.

A sample of a completed tube network is shown in Fig. 2. This network represents the pore structure in a two-dimensional slice through a three-dimensional particle array. In the sample shown, and in Fig. 1, the particles are uniform spheres. They appear to have nonuniform sizes only because of varying positions in the out-of-plane direction. The volume within this collection of tubes is the domain of the network model on which the conservation equations are solved.

CONSERVATION EQUATIONS

The transport equations governing fluid motion and species transport in a network model are much simpler than those usually encountered in multidimensional transport in porous materials. The reason for this is that all complexities of the pore geometry are explicitly described by the network itself. Phenomena such as reduced diffusivities due to the presence of a solids fraction and both longitudinal and transverse dispersion arise naturally as a consequence of the network geometry. As a result, these porous media transport phenomena, described by empirical correlations in conventional continuum models, are addressed in a network model on a first-principles basis, or nearly so.

For the isothermal transport of a species i through the tube network, conservation of mass is given simply by

$$V_k \frac{d}{dt}(\rho_k f_{i,k}) = \sum_{j=1}^{3} q_{j,k} \bar{f}_{j,k} - S_k \qquad (1)$$

where V_k is the portion of tube volume associated with node k, ρ_k is the fluid density at node k, and $f_{i,k}$ is the local species fraction. The summation on the right of Eq. (1) is a sum over the species transport rates from the three tubes connected to node k, and $\bar{f}_{j,k}$ is the mean species concentration in each tube. The final term on the right of Eq. (1) accounts for any sources or sinks do to surface or homogeneous reactions.

Momentum equations for the network model are likewise much simpler than those for continuum models of porous materials. Here, for low Reynolds number flows, the mean fluid velocity is related to the pressure gradient by conventional tube or channel correlations.

$$q_{j,k} = -\rho \frac{\bar{\delta}_{j,k}^3}{24} \frac{\Delta p_{j,k}}{\ell_{j,k}} \quad \text{or} \quad q_{j,k} = -\rho\pi \frac{\bar{\delta}_{j,k}^4}{64} \frac{\Delta p_{j,k}}{\ell_{j,k}} \tag{2a,b}$$

$\Delta p_{j,k}$ is the pressure drop across the tube joining the j and k nodes, ℓ is the tube length, and $\bar{\delta}_{j,k}$ is the equivalent tube aperture yielding the correct mean flow rate. Equivalent apertures are discussed further in the following section. The first of these relations applies to a two-dimensional channel, appropriate for flow in two-dimensional geometries, while the second applies to a circular tube, appropriate for three-dimensional particle arrays.

To solve the governing transport equations, pressures are imposed on two external surfaces of the network domain. The other two boundaries are made impermeable by closing any tubes crossing these planes. Pressures for the tube network are then computed by solving Eq. (1) for each interior node. This system of coupled node equations is solved by a time marching algorithm. Using an appropriate equation-of-state relating the fluid pressure, temperature and density, either liquid or gas flows may be treated in this way. The algorithms for computing the pressure field are given in pages 35 through 48 of Appendix A.

Once the internal pressures and tube mass flow rates are computed, the permeability of the network is calculated by summing the flow contributions from each tube to obtain the total flow rate through the entire network. From this total flow rate, the fluid properties, size of the domain, and the specified boundary pressures, the macro-scale permeability of the medium can be computed. By letting tube diameters diminish as biomass accumulates or as channels become blocked by particulate fines, changes in the pore structure and the effect of the evolving structure on the flow rate can also be computed.

Finally, we note that Eq. (1) does not contain any contribution due to diffusive transport. Although this additional transport mechanism can be included in this manner, we have found that describing diffusive processes via tracer particles is generally a more direct means of utilizing the full capabilities of the network model. Tracer particle dynamics are addressed in a later section.

NETWORK SUB-SCALE MODELS

Although a network model resolves transport phenomena down to the particle scale, many important processes take place on still smaller scales. Diffusion and viscous dissipation, for example, both involve processes occurring at the molecular scale. Rather than explicitly modeling the details of molecular interactions, these sub-scale phenomena are treated here in the conventional continuum fashion. Further, by averaging the governing continuum equations over the channel cross-sections and then integrating over their lengths, closed-form expressions for effective transport properties of each tube segment are obtained. These permit computation of the full pressure and concentration fields using state variables only at the network nodes.

To account for sub-scale processes in the network model, we define four equivalent apertures relating the tube volume, effective permeability, diffusivity and fluid transit time to the tube length. The simplest of these is the equivalent aperture for tube volume, δ_V, defined by

$$V = \ell\,\delta_V \tag{3}$$

where ℓ is the tube length, and V is its volume. It is staightforward to show that in this case the equivalent aperture is given by

$$\delta_V = \frac{2}{\ell}\int_0^{\ell/2} \delta dz \tag{4}$$

where δ is the local tube aperture.

The second equivalent aperture is that of the permeability. In this case, the equivalent aperture for two-dimensional flow is defined by

$$q = -\frac{\delta^3}{12}\frac{dp}{dz} = -\frac{\delta_k}{12}\frac{\Delta p}{\ell} \tag{5}$$

where q is the constant volumetric flow rate through the tube, p is the local pressure and Δp is the total pressure drop along the tube. Note that we make no distinction here between compressible and incompressible flow. The reason for this is that each tube is very short, thus the ratio of the pressure drop to the mean pressure is always very small. In light of this, the effects of compressibility may be neglected on this scale. To solve for δ_k requires that the local pressure is integrated over the tube length to obtain the total pressure drop. Substituting that result into Eq. (5) then yields

$$\frac{1}{\delta_k^3} = \frac{2}{\ell}\int_0^{\ell/2} \frac{dz}{\delta^3} \tag{6}$$

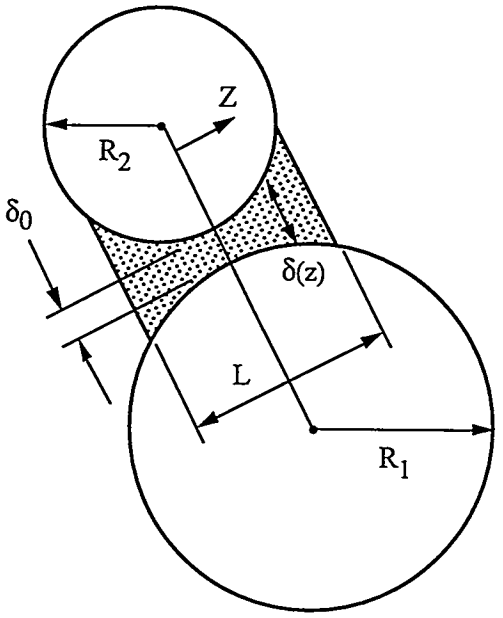


Figure 3. Diagram of a particle pair and flow channel. Equivalent apertures for pore volume, flow, diffusion, and through-channel transit time are computed using the channel geometry.

for the equivalent aperture providing the correct viscous forces within each tube.

The third equivalent aperture is that for the diffusivity. This is defined such that the constant diffusive transport rate, f, through a tube is correctly specified by

$$f = \delta D \frac{dc}{dz} = \delta_D D \frac{\Delta c}{\ell} \tag{7}$$

where D is the coefficient of binary diffusion, c is the local concentration of the diffusing species and Δc is the total variation of the concentration along the tube length. Now integrating Eq. (7) over the tube length to obtain the total variation in the concentration, and substituting that result back into Eq. (7) gives

$$\frac{1}{\delta_D} = \frac{2}{\ell} \int_0^{\ell/2} \frac{dz}{\delta} \tag{8}$$

for the equivalent tube aperture based on diffusion.

The final aperture to be defined is that for the mean fluid velocity or transit time. This yields the correct time a tracer particle is resident within a tube and so is useful in tracking particle motion within the network. In this case, the equivalent aperture is defined by

$$t = 2 \int_0^{\ell/2} \frac{dz}{u} = \frac{\ell}{\bar{u}} \tag{9}$$

where t is the tube transit time, and u and $\bar{u}$ are the local and mean fluid speeds, respectively. These are given by

$$u = -\frac{\delta^2}{12}\frac{dp}{dz} \qquad \text{and} \qquad \bar{u} = -\frac{\delta_u^2}{12}\frac{\Delta p}{\ell} \tag{10a,b}$$

Substituting Eqs. (10a) and (10b) into Eq. (9) and rearranging slightly yields

$$\frac{1}{\delta_u^2} = \frac{2}{\ell}\int_0^{\ell/2} \frac{\delta}{\delta_k^3}\, dz = \frac{\delta_V}{\delta_k^3} \tag{11}$$

Thus the equivalent aperture for mean fluid speed and transit time can be written simply in terms of those for the permeability, δ_k, and the tube volume, δ_V.

To apply these definitions of the four equivalent apertures, we must now take into account a specific particle geometry. Consider two two-dimensional particles having centers (x_1, y_1) and (x_2, y_2), and radii R_1 and R_2. As shown in Fig. 3, the local aperture between these particles is given by

$$\delta = \delta_0 + R_1 + R_2 - \sqrt{R_1^2 - z^2} - \sqrt{R_2^2 - z^2} \tag{12}$$

where the minimum aperture, occurring along the line joining the two centers, is

$$\delta_0 = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2} - R_1 - R_2 \tag{13}$$

and z is the distance measured in a direction orthogonal to the line of centers. Now taking

$$R_2 = R_1\,(1 + \epsilon) \qquad \text{and} \qquad z = R_1 \sin\theta \tag{14a,b}$$

and substituting these results into Eq. (12), the local aperture can be expressed in terms of only R_1, ϵ and θ.

$$\delta = \delta_0 + R_1 \left[\!\!\left[2 + \epsilon - \cos\theta - (1+\epsilon)\left[1 - \frac{\sin^2\theta}{(1+\epsilon)^2}\right]^{1/2} \right]\!\!\right]$$
$$\approx \delta_0 + R_1\left[1 - 2\cos\theta + \epsilon(1 - \sec\theta)\right] \tag{15a,b}$$

Note that the latter of these relations is based on a one-term expansion for small values of ϵ.

Substituting Eq. (12) into Eq. (2) and performing the indicated integration yields

$$\frac{\delta_V}{R_1} = 2\kappa + \epsilon - \frac{1}{2}\left[(1+\epsilon)^2 - \sin^2\theta\right]^{1/2}$$
$$-\frac{R_1}{\ell}(1+\epsilon)^2 \sin^{-1}\left(\frac{\sin\theta}{1+\epsilon}\right) - \frac{1}{2}\left(1 - \sin^2\theta\right)^{1/2} - \frac{R_1}{\ell}\theta \tag{16a,b}$$

for the equivalent volume aperture. The new parameter, κ, appearing here is given by

$$\kappa = 1 + \frac{\delta_0}{2R_1} \tag{17}$$

and in this case θ is evaluated at the angular limit of integration

$$\theta = \sin^{-1}\left(\frac{\ell}{2R_1}\right) \tag{18}$$

corresponding to the end of the tube segment.

Similarly, the equivalent aperture yielding the correct viscous drag is obtained by substituting Eq. (15b) into Eq. (6) and integrating the result. Using a tedious though straightforward change of variables, this gives

$$\frac{\delta_k^3}{\ell R_1^2} = 4\frac{\kappa^2 - 1}{f(\kappa,\theta)}\left[1 + \frac{3\epsilon I(\kappa,\theta)(\kappa^2-1)}{2f(\kappa,\theta)}\right] \tag{19}$$

where

$$I(\kappa,\theta) = \frac{1}{3(\kappa+1)}\left[\frac{\sin\theta}{(\kappa-\cos\theta)^3} - \frac{3h(\kappa,\theta)}{2(\kappa^2-1)} + \frac{2f(\kappa,\theta)}{2(\kappa^2-1)}\right] \tag{20}$$

where the functions $h(\kappa,\theta)$ and $f(\kappa,\theta)$ are

$$h(\kappa,\theta) = \frac{\sin\theta}{(\kappa-\cos\theta)^2} + \frac{3\kappa\sin\theta}{(\kappa^2-1)(\kappa-cos\theta)} + 2\frac{2\kappa^2+1}{(\kappa^2-1)^{3/2}}\tan^{-1}\left[\left(\frac{\kappa+1}{\kappa-1}\right)\tan\left(\frac{\theta}{2}\right)\right] \tag{21}$$

and

$$f(\kappa,\theta) = \frac{(2+\kappa^2)\sin\theta}{2(\kappa^2-1)(\kappa-\cos\theta)} + \frac{\kappa\sin\theta}{2(\kappa-\cos\theta)^2} + \frac{3\kappa}{(\kappa^2-1)^{3/2}}\tan^{-1}\left[\left(\frac{\kappa+1}{\kappa-1}\right)^{1/2}\tan\left(\frac{\theta}{2}\right)\right] \tag{22}$$

respectively.

Finally, we consider the equivalent aperture appropriate for computing diffusive transport through the tube network. Now substituting Eq. (15b) into Eq. (8) and again performing the integration gives

$$\frac{\delta_D}{\ell} = \frac{1}{g(\kappa,\theta)}\left[1 + \frac{\epsilon\psi(\kappa,\theta)}{2(\kappa+1)g(\kappa,\theta)}\right] \tag{23}$$

where

$$g(\kappa,\theta) = -\theta + \frac{2\kappa}{(\kappa^2-1)^{1/2}} \tan^{-1}\left[\left(\frac{\kappa+1}{\kappa-1}\right)^{1/2} \tan\left(\frac{\theta}{2}\right)\right] \tag{24}$$

and

$$\psi(\kappa,\theta) = \frac{\sin\theta}{\kappa-\cos\theta} - \frac{2}{(\kappa^2-1)^{1/2}} \tan^{-1}\left[\left(\frac{\kappa+1}{\kappa-1}\right)^{1/2} \tan\left(\frac{\theta}{2}\right)\right] \tag{25}$$

For the special case in which all particles within the particle array are the same size, the results above become greatly simplified. Rewriting Eq. (16) for $\epsilon = 0$ yields

$$\frac{\delta_V}{R} = 2\kappa - \left(1-\sin^2\theta\right)^{1/2} - 2\frac{R}{\ell}\theta \tag{26}$$

for the equivalent volume aperture. Similarly, Eq. (19) in this limit reduces to

$$\frac{\delta_k^3}{\ell R^2} = \frac{4\left(\kappa^2-1\right)}{f(\kappa,\theta)} \tag{27}$$

for the equivalent aperture for viscous fluid flow. Finally, the equivalent aperture for diffusion, given by Eq. (23) above, becomes

$$\frac{\delta_D}{\ell} = \frac{1}{g(\kappa,\theta)} \tag{28}$$

for this case of uniform particle size. As before, the angular limit of integration, θ, is taken as that corresponding to the tube length.

EFFECTIVE TRANSPORT PROPERTIES

The sub-grid models described above are intended for use in a network model generally capable of describing transport in disordered porous materials. We can, however, also apply these sub-grid relations directly to regular particle arrays. For such regular arrays, the geometry of the corresponding pore network is easily specified. In addition, the permeability and diffusivity have been computed by direct solution of the Navier-Stokes and diffusion equations for several regular patterns of two and three-dimensional particles [29,30,31]. Comparing the present results with

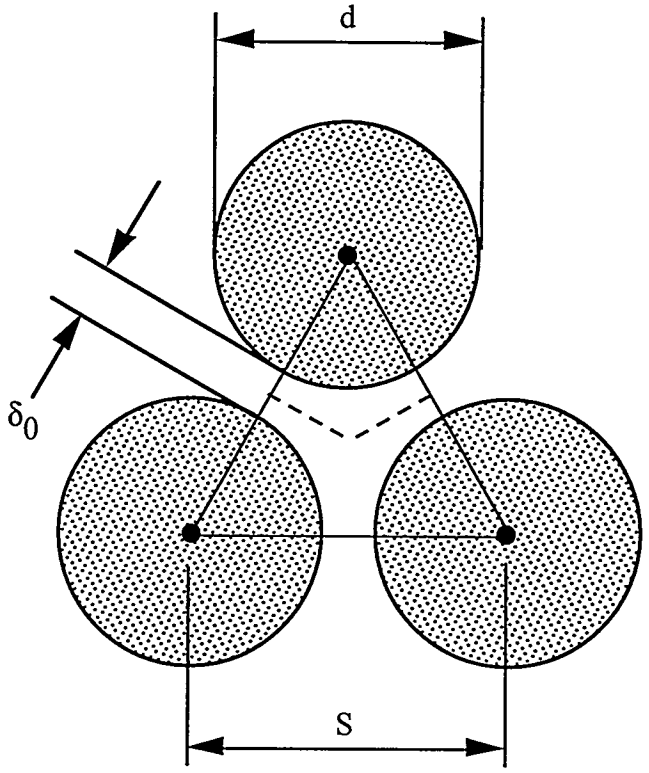


Figure 4. Unit cell of uniform hexagonal array of cylindrical particles. Particle size and minimum aperture determine porosity, diffusivity and permeability.

these numerical solutions provides a useful check on the accuracy of the network approach and on the range of applicability of correlations derived from the equations outlined earlier.

To this end, we now consider the simple problem of flow and diffusion through a regular hexagonal array of circular cylinders. As shown in Fig. 4, the particle size and geometry of the unit cell uniquely determine all transport properties of the array. From the definitions of the equivalent apertures, the effective permeability of this array is given by

$$k = \frac{1}{12}\frac{\delta_k^3}{h\sqrt{\tau}} \tag{29}$$

where $h = \sqrt{3}S/2$ is the height of the unit cell, and $\tau = 4/3$ is the tortuosity for flow from left to right in the geometry shown. Again, δ_k is the equivalent aperture for viscous flow. Using Eq. (27), this result may be expressed as

$$k = \frac{1}{12}\frac{\left(\kappa^2 - 1\right)}{f(\kappa,\theta)}\frac{\ell d^2}{h\sqrt{\tau}} \tag{30}$$

where $f(\kappa,\theta)$ is given by Eq. (22). Again from the geometry we obtain

$$\frac{\ell}{h} = \frac{2}{3} \quad \text{and} \quad \kappa = 1 + \frac{\delta_0}{d} = \sqrt{\frac{1-\phi_0}{1-\phi}} \tag{31a,b}$$

where ϕ is the porosity (void volume fraction), and $\phi_0 = 1 - \pi/2\sqrt{3} \approx 0.093$ is the porosity at the percolation threshold. The percolation threshold is the condition at which interconnected pores just marginally span the material sample of interest. Also from geometry, the angular limit of integration is

$$\theta = \sin^{-1}\left(\frac{\ell}{d}\right) \quad \text{where} \quad \frac{\ell}{d} = \frac{\kappa}{\sqrt{3}} \tag{32a,b}$$

Now defining a reference permeability as the area of the unit cell,

$$k_r = \frac{\pi d^2}{4(1-\phi)} \tag{33}$$

the normalized permeability may be expressed as

$$k^* = \frac{k}{k_r} = \frac{\phi - \phi_0}{3\sqrt{3}\pi f(\kappa,\theta)} \tag{34}$$

We note that exactly this result is also obtained for vertical flow through the unit cell of Fig. 4. The application of equivalent apertures to that problem is somewhat more difficult, however, since the unit cell for flow in that direction involves the confluence of two tubes into one.

A comparison between these results and an exact analytical solution to the problem [32] is shown in Fig. 5. For this simplified geometry of a regular hexagonal array, Eq. (34) agrees to within 15% for all porosities above the percolation threshold and below $\phi = 0.9$. Based on this agreement, we conclude that the expressions describing the equivalent aperture for viscous flow in two-dimensional channels should be suitable for network modeling of flow through disordered materials. Similar agreement has been obtained between the equivalent aperture formulas and exact solutions for two-dimensional square arrays and for the more complex problem of three-dimensional flow through regular arrays of spheres.

We now consider the use of equivalent apertures for computing the effective diffusivity of a regular hexagonal array. From Eqs. (8) and (28), the effective diffusivity may be written as

$$D^* = \frac{D_e}{D} = \frac{\delta_D}{h\sqrt{\tau}} = \frac{\ell}{hg(\kappa,\theta)\sqrt{\tau}} \tag{35}$$

where D_e is the apparent diffusivity in the porous array, and D is the coefficient of diffusion. This expression can be evaluated directly using the values of ℓ/h, κ, θ and τ given above, along with Eq. (24) for $g(\kappa,\theta)$. Again, although this result applies to diffusion from left to right in the geometry shown in Fig. 4, the same

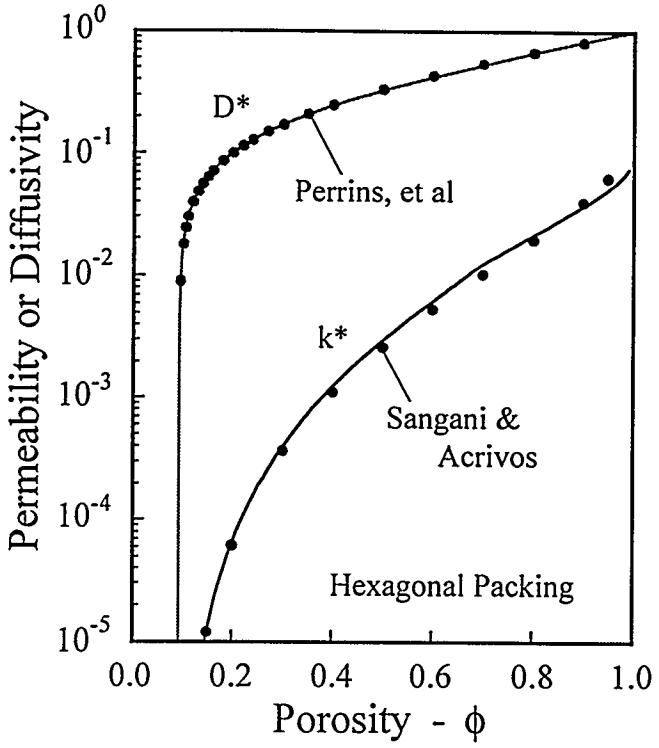


Figure 5. Comparison between network results and exact solutions from previous analyses of the normalized permeability and effective diffusivity for a regular hexagonal array of cylindrical particles.

result is obtained for diffusion in the vertical direction, and for that matter, in any arbitrary direction through the unit cell.

A comparison between this result and analytical solutions to the diffusion problem [33] is also shown in Fig. 5. In this case, Eq. (35) agrees to within 10% for all porosities above the percolation threshold and below $\phi = 0.8$. Again, a similar approach has been applied to other geometries with comparable agreement between the results of the network model and direct numerical solutions.

Although the diffusivity and permeability of a well ordered medium can be described analytically, numerical simulations are usually needed to determine the transport properties of random materials. To deduce the permeability of a particular network model, it is only necessary to set pressure boundary conditions on a pair of opposing faces and calculate the resulting flow rate. By seeding tracer particles into the flow and observing their motion it is then possible to observe the process of hydrodynamic dispersion that results from differences in fluid speed along different streamlines. The dispersivity of a given medium is influenced by the distribution of tube sizes and lengths, the degree of connectivity, and the degree of mixing that occurs at tube junctions. Dispersion also occurs on the scale of a single flow tube owing to differences in fluid speed between wall and center streamlines. All of these factors are accounted for explicitly in the network model by means of tracer particles.

PARTICLE TRANSPORT

Tracer particles may serve either as fictitious markers of the fluid motion or as physical particles of finite size. In the first capacity they are used to represent diffusive and dispersive contributions to the transport of reactive species carried by the mean flow [34,35,36]. In the latter role, physical particles of a finite size can be advected through the network to describe the advection, deposition, and accumulation of particles in the void space [37,38,39]. Blockage or partial blockage of individual tubes is straightforward to compute since the full geometry of the tube network is known and may be evolved in time. Thus, the reduction in permeability due to the relocation and deposition of biomass and native fines can be calculated from fundamental considerations.

To track the motion of tracer particles requires a knowledge not only of their streamline positions within tubes but also of their trajectories at nodal interconnections. Two basic configurations of nodes are possible: (1) a node having one in-flow and two out-flow tubes: and (2) a node having two in-flow and one out-flow tubes. These are the only possible configurations for a network constructed via Voronoi tessellation. In assigning particles to outflow tubes it is simplest to assume that all junctions are well mixed and to assign probabilities to the outflow channels and their streamlines based on their respective flow rates. However, it is generally much more realistic to require that particles follow continuous paths that smoothly interconnect the incoming and outgoing streamlines. That substantially more difficult approach is implemented in the present network model.

To compute particle motion through a network node, we assume a parabolic fluid velocity profile over the cross-section of each of the three tubes forming the node. Given the spatial position of a particle as it exits a tube, the node entrance streamline based on the parabolic velocity distribution can be determined. The corresponding node exit streamline can then be computed based on the total node in-flow and out-flow and knowledge of whether the node currently posses one or two in-flow tubes. Having computed the node exit streamline, the particle is placed at the correct radial position (in the correct exit tube, if more than one exit tube exists) again based on the parabolic velocity profile. Using this approach, real or tracer particles may be transported through the entire tube network following a single streamline through the repeated branching and confluence of tubes. For low Reynolds number creeping flows, typical of those in the applications of interest, turbulent transport of particles across streamlines does not exist. The only mechanism for this process is particle diffusion. It is this diffusion, along with the velocity profile within each tube and the variation in mean tube velocities, that gives rise to both longitudinal and transverse dispersion in flows in porous material.

Dispersion in a porous material is a complex process involving simultaneous flow and diffusion [40,41]. To model this process, we first compute the mean flow

field for the entire tube network. This yields the local fluid speed at each radial and longitudinal position within each network tube. We then inject a large number of particles at the inflow boundary and track their progress through the network for a fixed time. Particles are partitioned among tubes on the inlet boundary based on the total inlet flow rate and the contribution to this total from each inlet tube. This ensures that particles enter the network inlet tubes in correct proportions. Once an inlet tube is selected, the particle is placed at a radial position using a probability distribution that reflects the parabolic velocity profile. This ensures that particles entering a given tube are correctly distributed in accordance with local fluid speeds. Under these procedures, particles enter the network as though they were supplied from a reservoir of fluid containing a uniform particle concentration.

As the injected particles enter the tube network, they are advected by the local mean flow and diffuse about this mean speed. The diffusive portion of this transport is described by a noninterfering random walk [21,34]. At each time step, an advective displacement is computed from the local fluid speed and the size of the time step, δt. The time step may be constant or may be obtained by sampling a uniform random distribution. For the same time period, a random diffusive displacement, $\delta \ell_D$ is computed from the time step size and the specified diffusivity, D. This is given by

$$\delta \ell_D = \xi \sqrt{2D\delta t} \tag{36}$$

where ξ is a distribution function that may be unity, random or Gaussian. All three give very similar results, provided that the step size is adjusted such that the mean step size is consistent with Eq. (36). The direction of the diffusive step is then computed by sampling a uniform random distribution, and the combined advective and diffusive steps are taken. If the resulting particle position is outside the tube network, the step is recomputed.

Since all of the tracer particles advance with different speeds, they tend to spread apart as they traverse the medium. To quantify this longitudinal dispersion, each of the particles is transported through the network for a fixed period, t, and the final position of each is noted. Following the injection and transport of a large number of particles, the cumulative distribution of final particle positions is fit with an error function to obtain the mean and variance of the particle positions. The error function is used because it is the solution to the continuum dispersion equations. The dispersivity, D^* is then be calculated from the variance, σ^2 of the particle positions by

$$D^* = \frac{\phi}{D} \frac{\sigma^2}{2t} \tag{37}$$

where ϕ is the porosity of the medium. The dispersivity is a property of the material, and so should be independent of the time interval, t, provided that the interval is large enough to sample a statistically significant portion of the network.

The procedure above is used to compute longitudinal dispersion and the longitudinal dispersivity. Transverse dispersivities are computed by a similar method, except that particles are injected into only a single entrance tube. In this case, the particles are tracked and the final transverse position of each is noted. These positions are fit using a Gaussian distribution, and the transverse dispersivity is computed from the variance, again using Eq. (37).

A random walk is also used, in the absence a net fluid motion, to compute the effective diffusivity in the network model. As in the earlier simulations of hydrodynamic dispersion, particles are introduced into tubes along a vertical or horizontal line through the network. In this case, however, the starting line is generally centered within the medium since there will be no net displacement of the particle front. From their initial positions, the particles are again sent on random walks. After a specified time period, the effective diffusivity of the network is computed by matching a Gaussian distribution to the computed spatial distribution of the final tracer positions.

A number of options may be exercised in computing diffusivities. The computational algorithm permits either a random walk on the tube network or directly on the void volume defined by the particles comprising the granular material. Also, when computing diffusivities, the distinct contributions of ordinary and Knudsen diffusion may be determined by varying the mean diffusive step size relative to the characteristic pore diameter. Knudsen diffusion becomes dominant when the mean free path (diffusive step size) of the tracer particles become comparable to that of the pore size. In this regime, most diffusive steps result in collisions with a particle of the porous structure. Although Knudsen diffusion is not usually important in bioremediation applications, this capability of the network model has been employed in computing effective diffusivities for porous fiber preforms used in composites manufacturing by low-pressure chemical vapor infiltration.

Particle transport simulations are particularly advantageous in computing the transport of reactive chemical species [35,36]. Using minor variations on the methods above, species concentrations can be computed from particle concentrations during continuous particle injection. Particle lifetimes defined by reaction probabilities, can be used to account for both homogeneous and surface reactions. Surface reaction rates are especially easy to compute by this technique since the surface impingement rate, defined by a particle displacement to a region outside the tube network, is already monitored as a necessary part of the particle advective and diffusive motion. Details of the mathematical methods used in particle transport appear in pages 48 through 58 of Appendix A.

SAMPLE CALCULATIONS

To demonstrate the unique capabilities of a network model, we now present the results of calculations for several sample problems. These sample problems include the pressure field for an incompressible flow, permeability reductions due to uniform film growth on particles of a granular medium, particle-scale fingering and the associated longitudinal dispersion, and the effects of the Peclet number on transverse dispersion.

The first step in solving all transport problems using a network model is to compute the pressure field. This is done by solving the coupled continuity equations for all network nodes by means of a relaxation technique, subject to the desired boundary conditions. The result is a two or three-dimensional spatial distribution of pressures. A sample pressure field is shown in Fig. 6. The horizontal axis in this plot is the spatial position along the direction of flow. The vertical axis is the normalized pressure, where the normalization is such that the inlet pressure is unity and the exit value is zero. Boundary conditions for this sample problem are fixed pressures on the inlet and exit and impermeable boundaries on the top and bottom of the domain. The inlet and exit conditions are imposed by identifying those nodes lying on these boundaries and assigning the appropriate value, which is then held fixed through computation. Conditions on the impermeable boundaries are imposed by identifying those tubes crossing the top or bottom of the domain, and assigning to these tubes an effective aperture of zero. In this manner, no flow may cross the top or bottom boundaries. These particular boundary conditions are frequently used because they permit a direct calculation of the directional permeability once the pressure and flow fields have been determined.

This plot shows one particularly interesting feature of a typical pressure field. Although the mean gradient of the pressure is always negative, corresponding to flow from the inlet toward the exit, local pressure gradients are sometimes positive. That is, on the scale of particles within a porous granular material, local fluid velocities may oppose the mean flow direction. This condition arises naturally in disordered materials and is important because such local variations in both the magnitude and direction of fluid speeds contribute significantly to the very large apparent diffusivities associated with longitudinal dispersion.

Another interesting feature of Fig. 6 is the degree to which the mean node pressures deviate from the linear gradient obtained from a continuum model. The gradient of mean node pressures is about 20% above the linear value near the inlet and about 20% below at the exit. This deviation from the continuum result arises because the permeability of the network is locally lower than the average value near the inlet and locally higher near the exit. Since the total flow rate through the network is the same at all axial positions, low local permeabilities give high pressure gradients, while high permeabilities give relatively lower gradients of the mean node

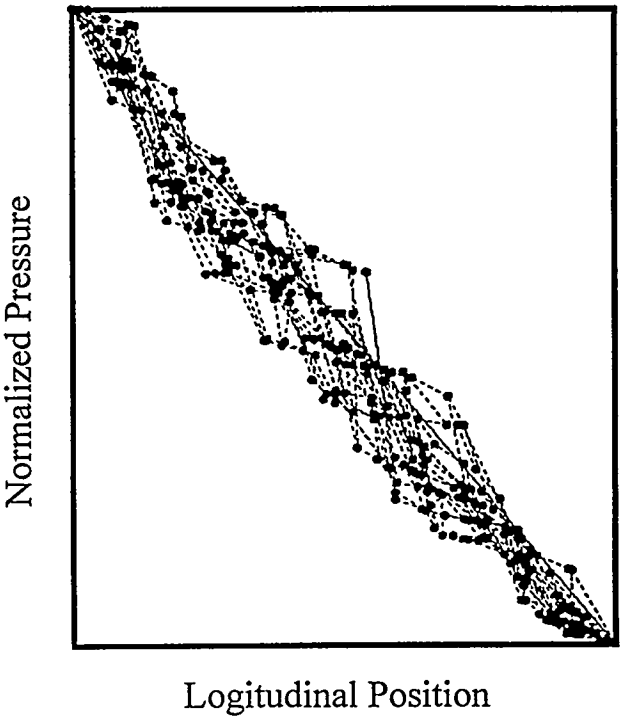


Figure 6. Normalized pressures at nodes inside a tube network. Dashed curves indicate interconnected nodes. The solid diagonal line shows the linear pressure gradient that satisfies the continuum equations for low Reynolds number flow of an incompressible fluid through a homogeneous porous medium.

pressure. This behavior is a result of the inherent nonuniformity of disordered porous materials. On larger domains, this effect is still more pronounced. This is important to the problem of bioremediation, since low permeabilities are associated with large specific surface area, and large surface areas lead to high contaminant retention. Thus regions most likely to require decontamination are also the most difficult to supply with the oxygen and nutrients needed for rapid treatment by this method.

We now consider the problem of the evolving pore structure and associated reductions in permeability due to accumulation of solids on particles of a granular porous solid. To generate the pore networks for this type of problem, we first generate a collection of particles by one of the three methods previously described. Then, a region of uniform thickness around each particle is excluded from the void space to account for that portion of the initial void occupied by the deposited material. This numerical process mimics that of biofilm growth on the surfaces of granular solids when the particle size is much larger than that of the microbe. Finally, the tube network is constructed about the particles and accumulated mass to obtain a network representation of the remaining void volume.

Three sample networks constructed in this way are shown if Fig. 7. Figure 7A represents the initial formation, while Figs. 7B and 7C represent the same collection

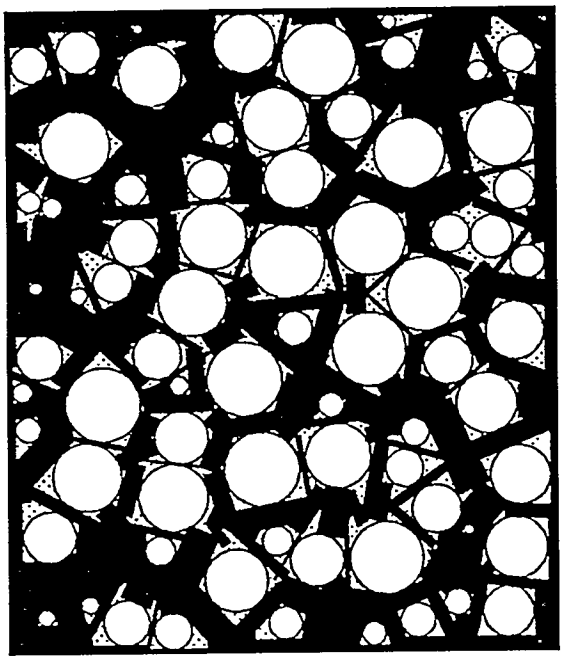
of particles with 33% and 66% of the initial void filled. The initial network (7A) at a porosity of 0.6 consists of 223 tubes and has a normalized permeability of about $k^* = 1.1 \times 10^{-3}$. When the porosity is reduced to 0.4, the resulting network (7B) still contains 166 tubes, but the normalized permeability has dropped by over an order of magnitude to only $k^* = 8.0 \times 10^{-5}$. This large reduction in permeability is due only in a small part to the fact that the remaining tubes have reduced diameters. The more important reason for this large effect is that the network void volume is losing connectivity. In the initial configuration, at a porosity of 0.6, over 97% of all the nodes are connected to two other nodes. At a porosity 0.4, only 37% of the nodes are still connected to two other nodes, over 50% are connected only to one, and about 10% are no longer connected to the network. Finally, at a porosity of 0.2, only 14% of the nodes remain doubly connected, 55% possess a single connection, and over 25% have become altogether isolated. It is this dramatic decrease in the number of interconnected pores that accounts for most of the large drop in permeability.

Despite the fact that the network still retains a large number of node connections at a porosity of 0.2, the permeability of the network shown in Fig. 7C is zero. At this porosity, the network is just below the percolation threshold, as a continuous path connecting the entrance and exit planes no longer exists.

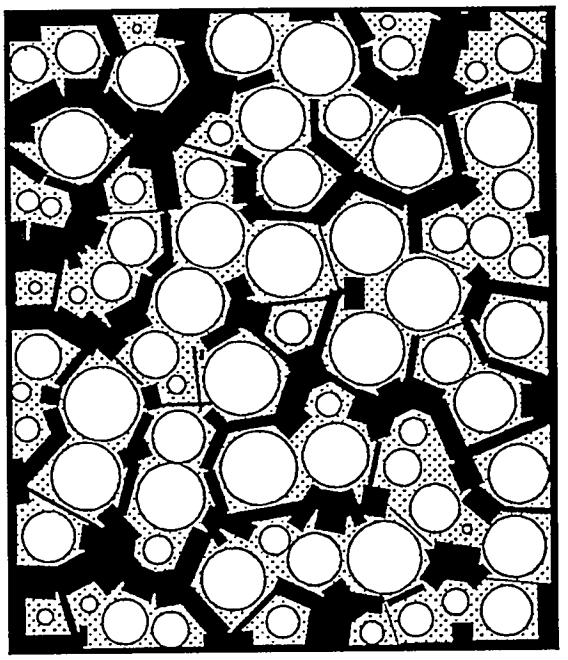
To illustrate the use of tracer particles in computing effective transport properties, we now consider the problems of longitudinal and lateral dispersion. Dispersion in a porous material is a complex process involving both flow and diffusion. Variations in local fluid velocities yield varying particle speeds as tracer particles traverse the pore network. Diffusion is important to this process because only by diffusion can particles move from one streamline to another. High diffusion coefficients give rise to a wider sampling of fast and slow streamlines in large and small pores, yielding smaller variations in average fluid speeds. Thus, contrary to intuition and to many statements made in the literature, an increase in molecular diffusivity leads to a decrease in longitudinal dispersivity.

Fig. 8 shows the instantaneous fluid interface during intrusion of a fluid into the pore network of a three-dimensional random packing of polydisperse particles. The interface is tracked across the network by a large number of tracer particles injected into the boundary between the two fluids. As the invading fluid fills progressively more of the pore volume, the interface roughens due to the varying mean fluid speeds along the various paths. This roughness of the advancing front is equivalent to a diffusion process in which the two fluids intermix along the plane of the intrusion front. This is not a true diffusion, however, and is referred to instead as dispersion.

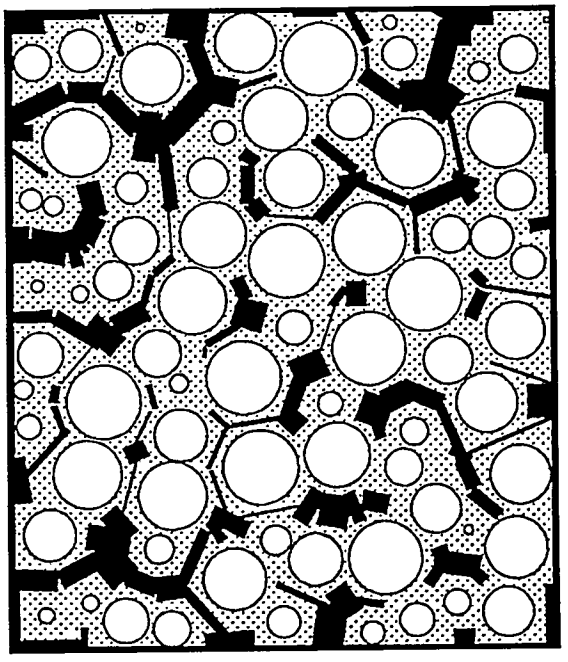
A pronounced feature of Fig. 8 is the finger-like structure of the fluid interface. Such structures are widely known to occur in flows in porous media when the viscosity of the invading fluid is lower than that of the fluid initially occupying the pore volume [42,43]. In that case, roughness of the interface results from an inherent



7A



7B



7C

Figure 7. Evolution of pore structure due to uniform accumulation on particles. 7A shows original pore structure, 7B shows 10% accumulation by total volume, and 7C shows 20% accumulation. The network of 7B has a permeability more than an order of magnitude below that of the original. The portion of the network shown in 7C is just below the percolation threshold.

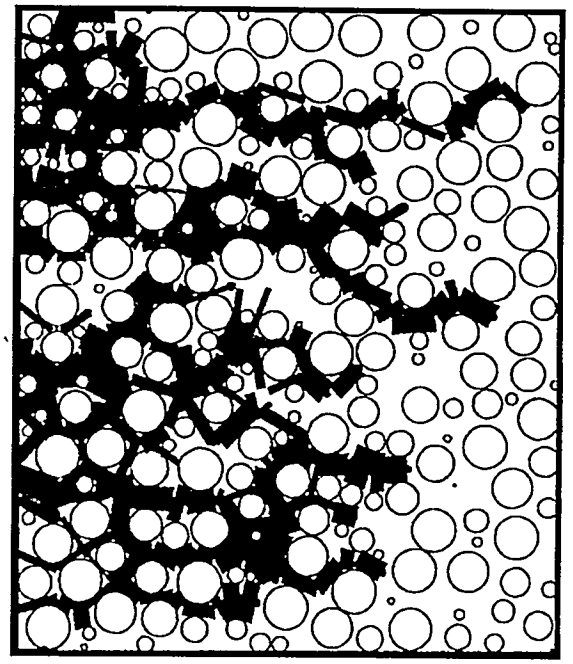


Figure 8. Particle-scale fingers in a pore network. Finger pattern results from local variations in permeability due to local variations in the size of interconnected pores. Unlike traditional viscous fingers, the pattern produced in a given pore network is largely deterministic in nature.

instability, and the resulting structures are known as Saffman-Taylor fingers [44]. The fingers in Fig. 8 do not have this origin. Instead, these fingers result only from the statistical nature of the distribution of pore sizes and connectivity of the pore network. For a given network, the formation of these fingers is almost entirely deterministic and depends only on the magnitude of the Peclet number indicating the relative importance of advective and diffusive transport.

Quantitative values of the dispersivity are extracted by analyzing the spatial distribution of the tracer particles used to map the intrusion interface. This is illustrated in Fig. 9. Here the final position of all tracer particles is shown on a slice through the particle array. The jagged solid curve is the cumulative distribution of these positions starting from the right boundary of the domain. The dashed curve is an error function, fit to the cumulative distribution in a least-squares sense by selecting the best values of the mean and standard deviation. The error function is used for this purpose because it is a solution to the continuum equations describing diffusion about the fluid interface. The dispersivity can be computed directly from the mean and variance obtained from this fit by the relation $D^* = \sigma^2/2t = \bar{u}\sigma^2/2\bar{x}$, where $\bar{u}$ is the mean fluid speed, σ^2 is the variance, and $\bar{x}$ is the mean particle position. Note that the very good agreement between the cumulative distribution

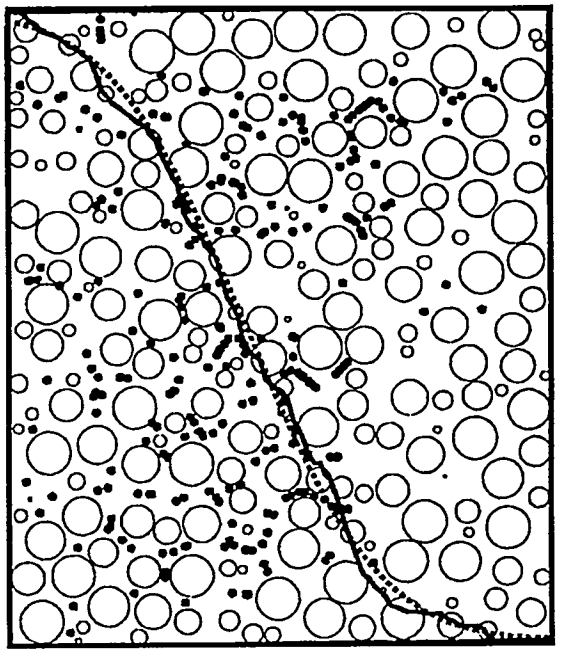


Figure 9. Tracer particle final positions. Particles are injected into the left boundary and carried by the mean flow for a specified period. Fitting the cumulative distribution of their final positions (dots and solid curve) using an error function (dashed curve) yields the dispersivity of the network.

of the particles positions and the error function fit indicates that dispersion in the network does indeed mimic a diffusion process.

The last sample problem concerns lateral dispersion. This is an important process in both bioremediation and contaminant transport since it strongly influences the vertical and lateral extent of the plume formed as fluids are transported downstream of a source. As with longitudinal dispersion, lateral dispersion involves a coupling between advective and diffusive transport. To examine this process, we have again computed the moving interface between two fluids during fluid injection. This time, however, the fluid is injected into a single tube on the left boundary of the network, rather than along its entire length. This is illustrated in Fig. 10. As before, a large number of particles are initially placed at the fluid interface. These are then carried into the network by the mean flow.

The results shown in Fig. 10 are for a special case in which there is no diffusion of the tracer particles between streamlines. In this case, lateral spreading of the plume is limited to a few pore diameters above and below the point of injection. The reason for this is that all of the particles are confined to the streamline on which they were injected. For low Reynolds numbers there is relatively little mixing of streamlines, even in highly disordered materials, so there is no mechanism to produce significant lateral spreading of the plume. As with longitudinal dispersion, a quantitative

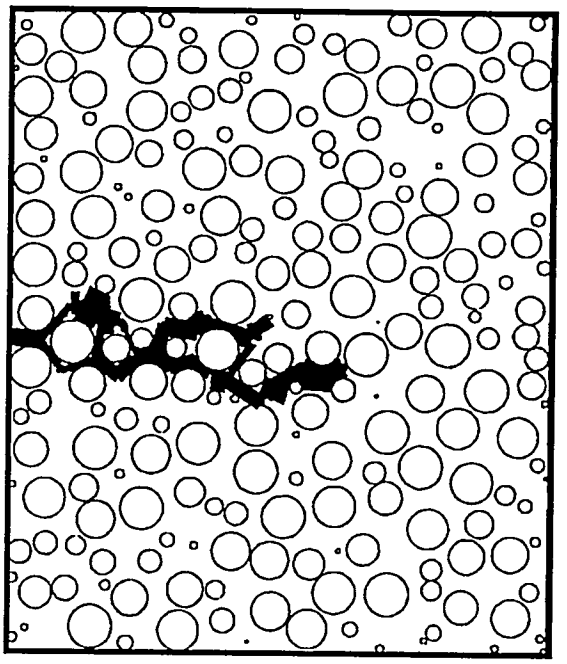


Figure 10. Particle-scale lateral dispersion in a pore network. At high Peclet numbers, lateral dispersion is limited because species do not move readily across streamlines within the pore volume. Results shown are for asymptotically large Peclet number.

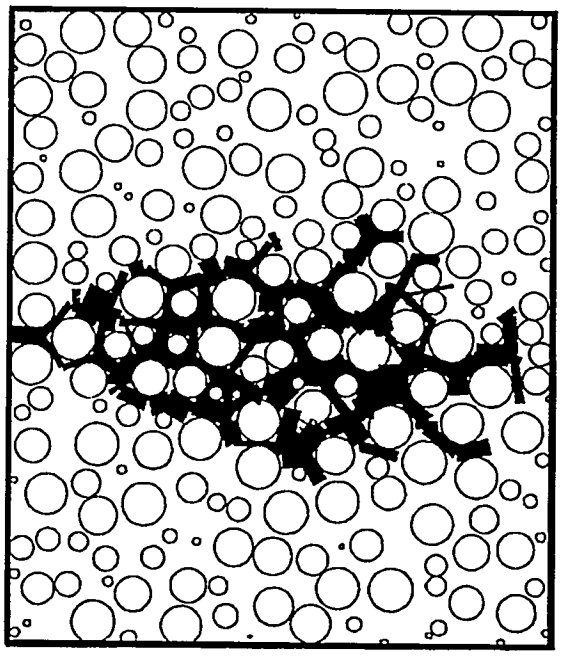


Figure 11. Lateral dispersion at low Peclet number. Large coefficient of diffusion allows tracer particles to cross streamlines and follow mean flow into an increasing lateral extent of the network. Results shown are for $\mathrm{Pe} = 1$.

estimate of the lateral dispersivity can be obtained by fitting the distribution of final particle positions within a slab vertical slab, using in this case a Gaussian profile.

In contrast to longitudinal dispersion, lateral dispersion becomes more pronounced when particles are allowed to diffuse between streamlines. This is illustrated in Fig. 11. Here, the intrusion interface is tracked through the same network used for Fig. 10. In this case, however, the coefficient of diffusion is set to a value to give a Peclet number based on the pore diameter of $\mathrm{Pe} = \rho \bar{u} d / D = 1$. The result is a dramatic increase in the extent of the lateral spread of the plume. The top and bottom boundaries of the plume now grow away from the centerline in proportion to the square-root of the longitudinal distance from the injection point. Note that the larger longitudinal extent of the plume is due to longitudinal dispersion, which is also present here but was absent in the results of Fig. 10.

It is important to recognize that the large lateral extent of the plume in Fig. 11 does not result directly from diffusion. For the diffusion coefficient used to obtain $\mathrm{Pe} = 1$, the maximum lateral extent of the plume would be only about half as large if diffusion were the only mechanism for lateral transport.

LABORATORY APPARATUS

The basic experimental approach for investigating deposition of fine suspended solid particles during fluid flow through a porous media was to determine the increases in the local hydraulic gradients within the porous media caused by the deposition of particles. These particles accumulate on the surfaces of the porous material over a considerable depth compared to the dimensions of a typical pore. Thus, pressure gradients are distributed over a relatively large distance within the porous media rather than being localized, e.g., at the surface of a filtering element or plate. The experimental protocol was to measure and record the local pressure distributions within the porous filtration media as a function of time. These data were then used to calculate the hydraulic gradient as a function of position in the packed bed. The experimental variables included the dimensions of the packing material used to create the porous media, the flow rate of the suspension, and the concentration of particulate material. Another objective of this work was to determine the local loading of deposited suspension that caused the observed increases in hydraulic gradients.

A schematic diagram of the experimental apparatus is shown in Fig. 12. An aqueous suspension was pumped from a continuously stirred reservoir to a cylindrical packed column that was operated in the upflow mode. Tubing ports along the axis of the column were connected to a differential pressure gauge to measure the

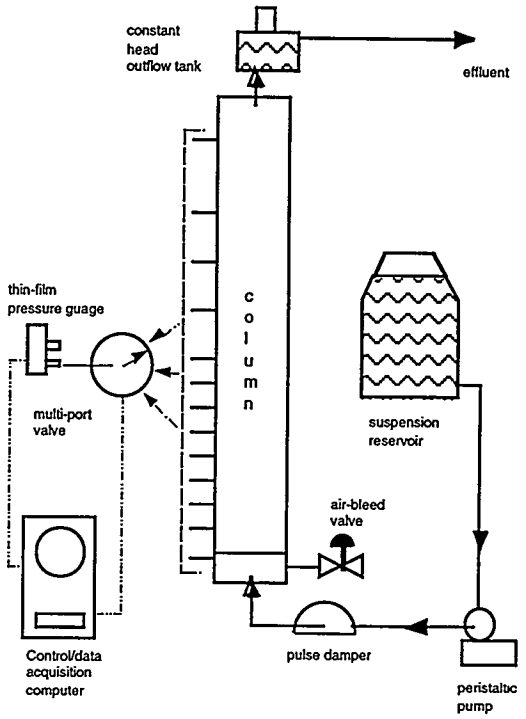


Figure 12. Diagram of experimental apparatus. Suspension is pumped through bottom of column against constant pressure of the reservoir at the top. Pressures are measured along the length of the column.

local hydraulic pressure relative to the prevailing atmospheric pressure in the laboratory. These pressure data were recorded and stored digitally during the course of an experiment. The liquid exited from the column by overflowing from a small tank that served to provide a constant hydrostatic head during the experiment. Photographs of the experimental apparatus are shown in Figs. 13 and 14..

The granular material that filtered the suspension was packed into cylindrical columns fabricated from acrylic tubing. The columns had an inside diameter of 50 mm (2.0 in.) and were approximately 0.51 m long. The packing material rested on a stainless steel wire mesh that was supported by a narrow ring of acrylic plastic held in place by a flange at the bottom (inlet end) of the column. This arrangement made virtually all of the column cross-section available for flow.

The detailed view of a packed column in Fig. 14 shows the arrangement for monitoring pressure during the flow experiments. A series of ports were drilled in the side wall of the column to allow access for measuring pressure. The pressure ports were spaced 10 mm apart near the inlet end of the columns, 20 mm apart in the center section, and 40 mm apart near the outlet (top end). The ports were spaced more closely near the inlet end as pressure gradients were expected to be largest there. The pressure ports consisted of stainless steel syringe tubing with Luer-Lok adapters that were used to connect the ports to the pressure-sensing device. The openings of the syringe tubes were aligned along the axis of the column. A fine piece

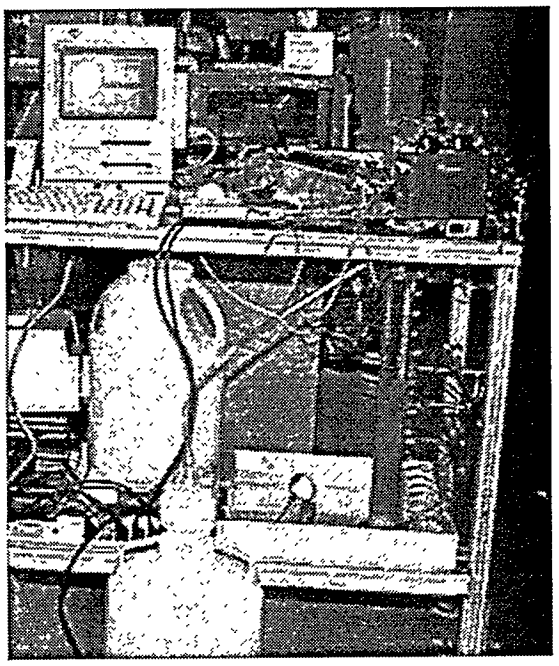


Figure 13. Photograph of the apparatus used to study flow in porous media, showing the packed bed column, reservoir, pump, data acquisition computer and pressure measuring system.

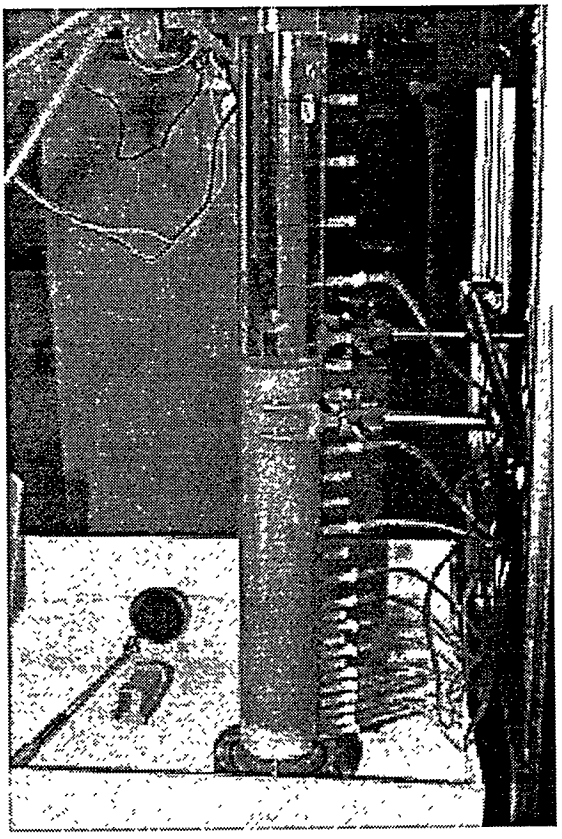


Figure 14. Photograph of a packed bed column as used for filtration experiments showing arrangement of the pressure monitoring ports. The white material at the bottom of the column is a deposit resulting from deposition of fines from a suspension.

Packing Material	Diameter (μm)	Mesh Size
P-170 Spheres*	300-450	40-50
A-055 Spheres*	500-600	30-35
Ottawa Sand**	600-850	20-30
A-150 Spheres*	1400-1700	12-14

* Potter's Industries, Inc., $\rho = 2.45 - 2.50$ gm/cc
** Fisher Scientific Co., $\rho = 2.62$ gm/cc

Table 1. Dimensions of the packing materials used for the filtration experiments.

of stainless steel wire was inserted into each of the syringe tubes to prevent intrusion and clogging by the packing material. As each monitoring port tube was necessarily filled with water to equalize the hydrostatic head before flow was initiated, the time response to changes in pressure were slowed somewhat by the reduction in cross-sectional area due to the inserted wire. However, pressure changes typically occurred quite slowly during these experiments, and the configuration used here responded to step pressure changes within 10 to 15 seconds.

Two types of materials were used to pack the filtration beds. The sizes of these packings are summarized in Table 1, where the particle size refers to the mean diameter. The primary packing material consisted of several grades of solid spherical beads of soda-lime glass (Potters Industries, Inc., Valley Forge, PA) that are classified into relatively narrow size ranges. Three sizes of spheres were used to provide a range of particle diameter that varied by a factor of about four, as indicated in Table 1. The second type of material was Ottawa sand (Fisher Scientific Corp., Pittsburgh, PA). It is a naturally-occurring silica sand that has been classified into a narrow size range of 600 to 850 μm (diameter), which corresponds to 20-30 mesh fraction. The individual grains of sand are generally ellipsoidal in shape. The complete specifications of Ottawa sand are given by ASTM-C 778-80a.

The columns were packed by gradually adding weighed amounts of a given packing material to a column filled with water to avoid trapping air. As the beads settled, the column was agitated by tapping to ensure a uniform packing distribution. The uniformity of packing was subsequently confirmed by measuring the hydraulic gradient during flow of deionized and filtered water and to verify that the gradient was uniform.

A peristaltic pump was used to supply a constant flow rate of suspension during these experiments. The suspension was pumped using a Masterflex Model 7523 peristaltic pump (Cole-Parmer Instrument Co., Vernon Hills, IL). Flow rates up to 270 milliliters per minute (ml/min) could be achieved. The flow rate was determined from the pump rotation speed, rather than in-line measurement, to avoid interference between the suspended particles and a flow sensor. The pumping rate was set by a digital speed control and was reproducible to $\pm 2\%$. Flow rates were calibrated by collecting known volumes of liquid during measured time intervals over the entire range of flow rates to be investigated using a variety of tubing sizes compatible with the pump heads.

Pulsations from the peristaltic pump were reduced, but not completely eliminated, by an in-line reservoir "pulse dampener," Cole-Parmer Instrument Co., Vernon Hills, IL) that established a trapped liquid/gas interface between the pump and the inlet to the column. This device required approximately 20 ml of liquid holdup and did not cause any loss of the suspended material in these tests. The amplitude of pulsations from the pump were also reduced quite effectively by using the smallest tubing diameter in the pump head that was capable of providing the desired flow rate. As smaller tubing required greater rotational speeds to achieve a given flow rate, the relatively high frequency of the pulses was found to reduce the peak-to-peak amplitude of pressure variations. The data acquisition system, described below, further reduced the influence of pulsations by using an averaging procedure to collect data. Experiments with clean water confirmed that hydraulic gradients could be measured accurately in the presence of larger pressure pulsations than actually occurred during filtration experiments.

The pressure measurement system was designed to determine relatively small hydraulic gradients and thus precise measurements of local pressures throughout the column were necessary. The measurement technique was based on eliminating the hydrostatic component of pressure, thereby increasing the resolution with which pressure changes due to fluid flow and, subsequently, the effect of particle deposition, could be determined. Measurements were made with thin-film pressure transducers (Omega Engineering Inc., Stamford, CT, Models PX-162 and PX-164) and water-filled manometers. The differential pressure transducers had ranges from 0 to 5 in. (water) to 0 to 27 in. (water) and provided electrical output signals that could be interfaced with the digital data acquisition system. The liquid manometers were used for baseline measurements of the hydraulic gradients during flow of clean water, rather than flow of suspensions.

Each pressure port was periodically connected to the pressure transducer by a computer-controlled multi-position valve (Valco Instruments, Houston, TX). The valve ports were connected sequentially, starting each cycle with the ports at the upper end of the column, having the lowest differential pressure, and stepping to the inlet port, having the largest differential pressure. This procedure minimized the

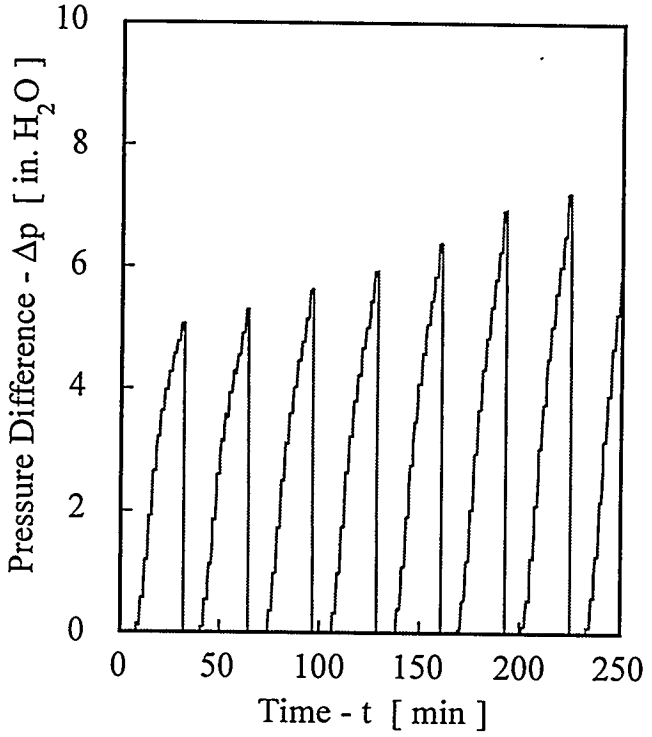


Figure 15. Representative data output showing the pressure distribution in a packed column during deposition from a suspension of fine clay particles.

offset inherent in the movement of the free surface of liquid between the manometer tubing and the valve/transducer interface. The first position of the valve was open to the atmosphere so that each cycle of pressure readings could re-establish an atmospheric (zero) reference pressure. Pressure readings were corrected for the slight displacement of the water-air interface in the manometer tubing by a calculation feature in the Workbench software. In addition, a time-averaging scheme in this software was used to minimize small fluctuations in pressure caused by the pump prior to capturing the data. The valve cycle was set to wait for one minute at each port, resulting in a total cycle period of 16 minutes.

Data acquisition and recording were performed using the software application, Workbench (Omega Engineering Corp., Stamford, CT) , running on an Apple Macintosh SE computer. This software also provided the stepping control of the multiposition valve and the synchronizing signal to identify which location in the column corresponded to the pressure data that were recorded. Fig. 15 shows a typical display of the pressure data captured during several complete sequences of valve operation during a flow experiment. The stepped line indicates the values of pressure at various locations in the column. The axial separation of pressure monitoring ports along the column is not necessarily equal between all of these steps. It is evident that the small pressure pulses created by the pump are very well damped.

Aqueous suspensions of particles of kaolin clay in a buffer solution were prepared for the filtration experiments. The constituents were kaolin powder, (Mallinkrodt

Chemical Co., St. Louis, MO, food grade) which is hydrated aluminum silicate having the approximate formula $H_2Al_2Si_2O_8$–X H_2O. Aluminum sulfate, $Al_2(SO4)_3$–X H_2O, or "alum" (Mallinkrodt Chemical Co., St. Louis, MO, reagent grade) was used as the coagulant for the suspended clay particles. Sodium bicarbonate and potassium chloride were added to buffer the suspension to near a neutral pH and to provide ionic strength. The standard suspension was prepared in deionized water to produce final concentrations of 30 mg/l kaolin, 10 mg/l alum, 50 mg/l KCl and 42 mg/l $NaHCO_3$ [45]. Typically, concentrated solutions or suspensions of the individual constituents were gradually added to deionized water before an experiment and stirred strongly by mechanical or ultrasonic agitation for several minutes. The suspension in the reservoir was continuously stirred during the flow tests, however, the suspended particles required several hours to settle out when stagnant. Several filtration experiments were conducted using suspensions in which the concentration of the constituents was doubled.

Flow experiments were initiated using clean water, pumped at the same flow rate intended for the suspension. This enabled us to collect data for the hydraulic gradient of the clean packing and to verify that all the data channels were functioning properly. Flow of suspension into the column was started at the beginning of the switching cycle of the multi-position valve. The test was continued, replenishing the suspension reservoir as needed, for up to 9 hours.

EXPERIMENTAL RESULTS

Hydraulic gradients were determined using columns loaded with the various packing materials in order to verify that our measurements corresponded to those reported by other workers and to ensure that the experimental system was functioning properly. Flow rates were varied over a wide range to ensure the consistency of the measured permeabilities. The data for hydraulic gradients measured for flow of water in clean columns is presented in Table 2. The hydraulic gradient is given in units of hydrostatic head (inches of water) per unit length of packing (inches) and is nominally dimensionless [48]. The filtration, or Darcy, velocity was calculated based on the volumetric flow rate and the void fraction of a given packed column.

These data are also plotted in Fig. 16, in which the measurements done in this work, represented by solid symbols, are compared with data from the literature, which are shown as open symbols. A direct comparison can be made of our data for a large packing material (1400-1700 μm) and the data of Darby, et al [47] using the same glass beads. These data agree very well. Similarly, Hunt's data [45] for a slightly smaller packing (1190-1400 μm) display a somewhat greater hydraulic gradient at a given filtration velocity compared to the largest packing, as expected. Extrapolating Hunt's data for a smaller packing (495-589 μm) and the data from this work for Ottawa sand (600-850 μm) also yields good agreement. Fig. 16 illustrates

Data Source	Diameter (μm)	Velocity (cm/s)	Gradient
P-0170 Beads	300-450	0.017	0.195
"	300-450	0.026	0.281
"	300-450	0.034	0.381
"	300-450	0.043	0.490
Ottawa Sand	600-850	0.034	0.110
"	600-850	0.051	0.161
"	600-850	0.068	0.202
A-150 Beads	1400-1700	0.034	0.026
"	1400-1700	0.051	0.037
"	1400-1700	0.068	0.047
"	1400-1700	0.085	0.057
Darby [47]	1400-1700	0.180	0.1
Darby [46]	500-600	0.170	0.57
Hunt [45]	495-589	0.145	0.38
"	495-589	0.279	0.73
"	1190-1400	0.145	0.12
"	1190-1400	0.279	0.23
Hunt [45]	1190-1400	0.554	0.46

Table 2. Hydraulic gradients measured for flow of water in clean packed columns.

that the hydraulic gradients determined in this work were considerably smaller than those reported in the literature. The experimental apparatus used in our work is much more sensitive to small differential pressure changes during flow than the prior studies.

Several experiments were conducted to verify the ability of the experimental apparatus to measure the increases in local hydraulic gradients that result as fine particles deposited within the column. The parameters varied were the size of the packing material, flowrate, and concentration of the suspended particles. The smallest packing material, P-0170 glass beads (see Table 1), collected the suspended fines very effectively, resulting in relatively large pressure drops between the inlet region and first (1-cm) monitoring port. The standard suspension concentration tended to clog this packing material quite readily, even at flowrates of only 40 ml/min. The suspension was not distributed over a sufficient length of the column to permit meaningful determinations of the hydraulic gradient in this case. Conversely, the largest packing material, A-150 glass beads, did not collect enough suspended

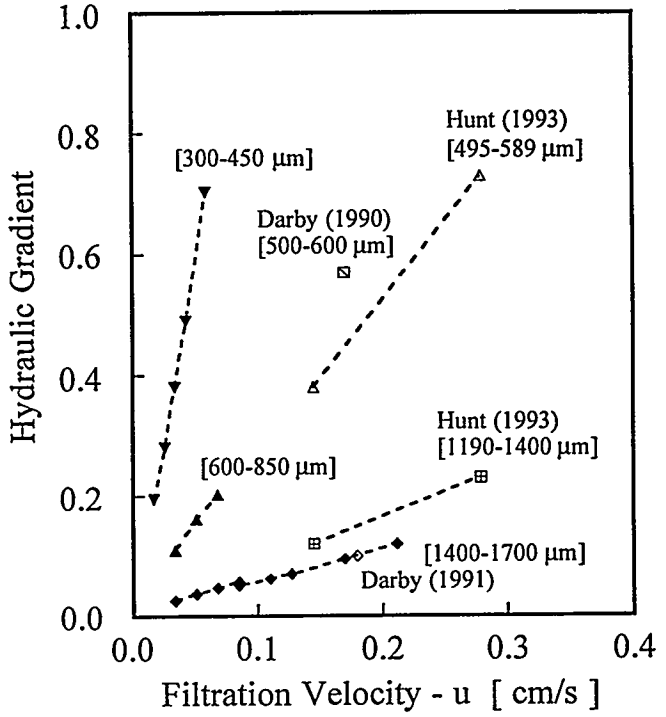


Figure 16. Hydraulic gradients measured in packed columns during flow of clean water.

fines during experiments lasting up to 10 hours to permit accurate measurements of the increases in hydraulic gradients. Even at the highest practical flowrate of 200 ml/min using a double concentration of fines did not deposit sufficient particulate for useful measurements.

Flow experiments with A-055 glass beads and Ottawa sand provided good examples of the utility of the experimental apparatus to measure hydraulic gradients during deposition of fines. The plot in Fig. 17 shows the increases in hydraulic gradient resulting during flow of suspended fines in the A-055 material. The units of hydraulic gradient are cm of water (head) per cm of column length in this plot. The ordinate indicates the axial position above the screen that supports the packing material, in centimeters. The filtration velocity was 0.085 cm/sec, which corresponds to a volumetric flowrate of 100 ml/min, and the concentration of the suspension was twice that specified in procedural section above. The dotted line indicates the mean hydraulic gradient for flow of water in a clean packed bed of A-055 glass beads at this filtration velocity. The values of the hydraulic gradient obtained for the upper part of the column (more than about 18 cm from the support screen) are essentially those of a clean column regardless of time. This result is expected as visual inspection confirmed that very few, if any, suspended particles appeared at the exit end of the packed bed. This result is also consistent with published reports that indicate that fines collect preferentially in the inlet section of a packed

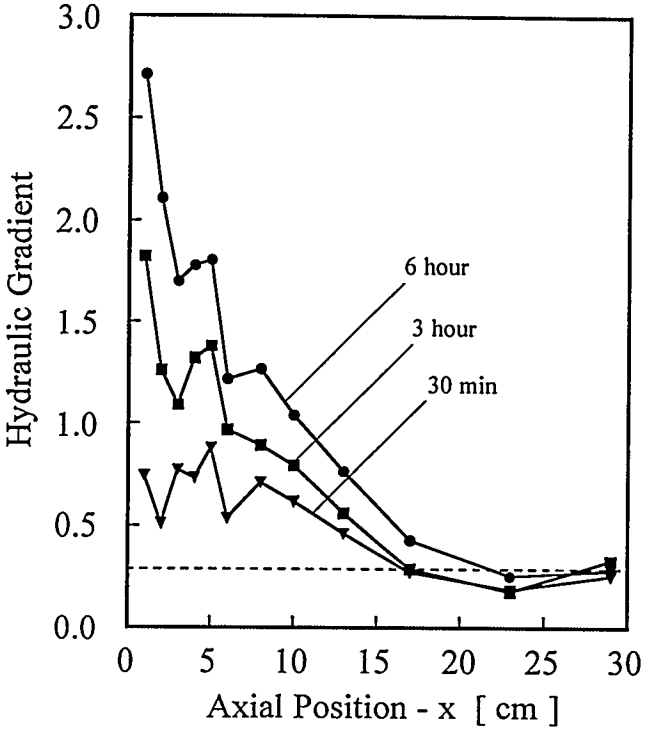


Figure 17. Observed increases in hydraulic gradient resulting from deposition of fines in a packed bed.

bed, under somewhat similar experimental conditions, rather than being distributed throughout the bed [45,46,47].

The data points and associated lines in Fig. 17 indicate that the hydraulic gradient increased as the experiment progressed and material collected preferentially in the entry region of the bed. The hydraulic gradient decreased with distance further from the inlet area, as expected. The anomaly in the data at positions 4 and 5 cm from the inlet could have been caused by clogging of the monitoring ports. A localized nonuniformity in the packing of the column may also have contributed to these anomalous results. Regardless, the expected trends in the data with regard to time and position in the bed were observed. When related to a mass balance of the total flux of fine particles into the column, these data are also consistent with literature reports, e.g. [45], that relatively small amounts of deposited particles can increase local hydraulic gradients by factors of 5 or more compared to the permeability of a clean column.

SUMMARY

The subsurface transport of nutrients and microorganisms is a key factor in determining the applicability of in situ bioremediation to waste site decontamination. One of the most important and least understood aspects of this transport process is the dramatic reduction in formation permeability resulting from the growth and accumulation of biomass. These processes, which may reduce permeabilities by three to four orders of magnitude, are strongly dependent on microstructural features of the host medium. Such features, including the pore size distribution and the degree of pore connectivity, cannot be explicitly accounted for in traditional site-scale continuum models. Instead, these processes must be investigated on scales comparable to those of the interstitial pore diameters.

To better understand the processes of transport and permeability reduction, we have constructed mathematical and laboratory models applicable to intermediate scales. These scales are large enough to encompass hundreds or thousands of pores, but still small compared to field operations. The mathematical model depicts flow and transport through a network of interconnected passages representing the pore volume of a granular material. This network model is sufficiently general to accommodate a broad range of transport processes in fully disordered materials, yet simple enough to permit derivation of closed-form relationships describing the permeability and effective diffusivity of regular particle arrays.

In contrast to most previous network models that simply interconnect randomly-placed tubes, our computational domain is generated by packing spheres or cylinders of a specified size distribution. This approach provides a more realistic representation of granular materials, soils, and sedimentary geologic media. Such attention to microstructural detail is especially important in modeling deposition processes, since reductions in permeability are very sensitive to pore geometry. The packing may be regular or may be constructed by one of several methods using statistical means to obtain varying degrees of disorder and varying packing densities. After fixing the size and location of all particles, a Voronoi tessellation is used to define the centerlines and junctions of the channels forming the network. The aperture of each channel varies with axial position along its length in accordance with the geometry of the bounding solid surfaces. To speed numerical solutions, analytical integration along each channel axis is used to define effective apertures used in calculating the pore volume, fluid speed, transit time, and the cross-sectional area for diffusion.

Although the network model is mainly intended for numerical simulation of transport in random packings, it can also be used to derive analytical expressions relating effective transport properties to the pore geometry. Closed-form expressions were derived for the effective permeability and effective diffusivity for transport through a hexagonal array of circular cylinders. These analytical results are

in good agreement with published solutions to the multidimensional equations describing Stokes flow and binary diffusion through a unit cell of the medium. Similar agreement has been obtained in applying this simplified version of the network model to more complex two and three-dimensional ordered media. In all cases, the effective transport properties are related to the fundamental geometric parameters used to characterize all permeable materials, including particle size, porosity, tortuosity, and the percolation threshold. In addressing random media and the more complex processes like dispersion and plugging, it is generally necessary to perform numerical simulations using the full capabilities of the model.

An important and powerful feature of this network model is its capability to simulate particle transport. Fictitious tracer particles can be used to compute effective diffusivities and dispersivities of disordered materials. In addition, particles of finite size can be used to simulate the transport and deposition of fines and the effect of such deposition on permeability. To compute dispersivities, particles are injected on the inlet boundary and transported through the network at the local fluid speed. During each time step of this deterministic motion, the tracer particles are also displaced by a random motion, simulating the effects of diffusion between adjacent streamlines within the pore volume. After a specified interval, the spatial distribution of the particle positions is fit with an error function or Gaussian profile to obtain the mean and variance of the particle positions. From these values, both the longitudinal and lateral dispersivity can be computed. In contrast to most previous work in which streamlines are assumed well mixed at each branching and confluence of channels, the present algorithm maps each streamline through these junctions. In the absence of diffusion it is therefore possible to trace each streamline within the network between the inlet and outlet boundaries. This avoids the artificial dispersion that can sometimes arise in network models.

Using this network model, permeability reductions during bioremediation can be simulated by computing a sequence of solutions for a fixed particle array in which particles of the array are coated by a layer of increasing thickness. In sample calculations presented here, we found that a reduction in porosity from 60% to 40% as a result of layer growth led to more than an order of magnitude reduction in permeability. Further reduction in the porosity to 20% led to a network below the percolation threshold. Such a dramatic reduction in permeability is not a direct consequence of narrowing in the larger channels, but rather results from a loss of interconnection within the pore network by the occlusion of many smaller passages.

Other sample calculations of flow in random granular materials revealed several interesting phenomena. In a rectangular domain having an imposed one-dimensional pressure gradient, we found regions in which the local pressure gradient was reversed and the direction of local flow opposed that of the mean pressure gradient. We also saw that the magnitude of the associated lateral pressure gradients were nearly 20% of that in the direction of mean flow. These deviations from the one-dimensional

continuum behavior are a consequence of disorder and heterogeneity. Such large variations in the pressure and velocity fields contribute substantially to macro-scale dispersion.

Experimental studies were conducted to investigate permeability reductions by the accumulation of fines. The apparatus developed for this purpose demonstrated the capability to make measurements of small, local pressure variations within a packed column at relatively low flow rates. This apparatus also enabled improved spatial resolution of permeability reductions within a column, as compared with previous systems described in the literature. Experiments with flow of clean water verified that our results agreed well with published data. Similarly, an experimental capability to measure reductions in permeability due to the deposition of fines during the flow of suspensions was demonstrated. In this series of experiments, permeability reductions were measured over a range of conditions in which the flow rate, properties of the fines suspension, and size and size distribution of the granular packing materials were varied.

One important goal in this program was to compare the measured and calculated permeability reductions for both fines deposition and biofilm growth. Out of this comparison, we intended to benchmark the simulations and develop constitutive relations describing permeability reductions. This goal was not achieved. Due to problems in writing SOPs for biologically active agents in the wake of the DOE Tiger Team visit and due to the relocation of personnel and the apparatus to the new IMTL building, the schedule for experimental work slipped significantly. This did not allow time, within the span of the program, to achieve these last goals. We have attempted to complete this portion of the work since that time, but this also has not been successful.

Despite these problems, we have already made use of several of the techniques and capabilities developed here in areas unrelated to bioremediation. The permeability and effective diffusivity of ordered and nearly-ordered carbon fiber arrays have been computed in support of an ARPA-funded program on the rapid densification of carbon-carbon composites. This manufacturing process shares with bioremediation the problem of formation blocking, leading to long processing times and very high cost. The Voronoi tessellation algorithm developed for generating our tube network has also been used to generate a structural skeleton for modeling the solid mechanics of propellant fragmentation in an MOU-funded study of propellant recovery by temperature cycling and for modeling the solid mechanics of foams in a Sandia CRADA with Dow Chemical Corporation. Finally, the network model is now being considered as a platform for modeling the transport and adsorption in micro-porous materials used as gas separation and storage devices.

ACKNOWLEDGMENT

The authors wish to thank R. S. Larson for his assistance in integrating several of the expressions used in computing effective transport properties. The assistance of B. C. Long in constructing and operating the experimental apparatus is also gratefully acknowledged.

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APPENDIX A - SOURCE LISTING OF PROGRAM BIOREM

BIOREM$MAIN

```
00001   C
00002         DIMENSION X0(500),Y0(500),SL(500)
00003         DIMENSION XX(131),YY(131),DDX(500),DDY(500)
00004         DIMENSION XS(500),YS(500),IPRM(12,500),LPRM(12,500)
00005         DIMENSION RADI(500),DIAM(500),HITE(500),DIAM0(500),HITE0(500)
00006         REAL LBON(12,500),LSID(12,500),AREA(500)
00007         DIMENSION XSID(12,500),YSID(12,500),DONE(500)
00008         DIMENSION PERI(500),APRX(500),APRY(500)
00009         REAL LOADR,LOADL,LOADT,LOADB,LBOUN(200),LOADX,LOADY
00010         INTEGER FSID(20),JB(200),NSID(500),NORM(4)
00011         DIMENSION WORK(4,500),IDBC(500),LBC(500)
00012   C
00013         INTEGER IDNOD(12,500),NODAR(11,1500),IDTUB(12,500),TUBNOD(4,1500)
00014         INTEGER KBLOC(1500), NNBC(4), NBID(4,200), IPIKT(3), TBID(4,200)
00015         REAL XNOD(1500),YNOD(1500),TUBAR(15,1500), FLO(3), APORE(1500)
00016         REAL XBA1(2),YBA1(2),XBA2(2),YBA2(2),XB(500),YB(500)
00017         REAL FREQ(500), XYNPAR(4,1500)
00018         REAL DNEIGH(18,500), DBOX(500)
00019         REAL DPER(1500), DDIF(1500), DVOL(1500), ARRTIM(1500)
00020         REAL XAA(3,3), RHS(3), XTU(1500), YTU(1500), RTU(1500), QHS(3)
00021         REAL XHS(3)
00022         REAL DETA, DETX, DETY, DETR
00023         INTEGER INEIGH(18,500), JBLOK(1500)
00024   C
00025         REAL*8 PRES(1500),PRESO(1500),DPRES(1500),DOTM,PSUM
00026         DIMENSION DX(1),DY(1)
00027         DIMENSION FX(1),FY(1),SMAX(1,1)
00028         DIMENSION TEM(1),DTEM(1),SSMX(1),FIDL(1),SIDL(1)
00029         DIMENSION XSOLD(1),YSOLD(1),DXOLD(1),DYOLD(1)
00030         DIMENSION UX(1),UY(1),UXOLD(1),UYOLD(1)
00031         DIMENSION AA(1,1),BB(1),RES(3),WX(1),WY(1)
00032         INTEGER IDS(1),IPOP(1,1),SED,SED0,JPOP(1,1),IWORK(1)
00033         DIMENSION VTRACE(1500)
00034   C
00035         REAL MAS,HGT,KMOD,KBLK
00036         COMMON XXX
00037         COMMON /BLKQ/ ALOGMU,ALOGSIG,ZZZ
00038   C
00039         DATA (NORM(I),I=1,4) /-1, 1, 1, -1/
00040   C
00041   C   NODAR (K,IDN)
00042   C     1: NUMBER OF ADJACENT NODES AND/OR CONNECTED TUBES
00043   C     2: NODE NUMBER OF ADJ NODE 1
00044   C     3: NODE NUMBER OF ADJ NODE 2
00045   C     4: NODE NUMBER OF ADJ NODE 3
00046   C     5: TUBE NUMBER JOINING NODE 1
00047   C     6: TUBE NUMBER JOINING NODE 2
00048   C     7: TUBE NUMBER JOINING NODE 3
00049   C     8: BOUNDARY NUMBER OF NOD IDN
00050   C     9: PARTICLE NUMBER 1
00051   C    10: PARTICLE NUMBER 2
00052   C    11: PARTICLE NUMBER 3
00053   C
00054   C   TUBAR (K,IDT)
00055   C     1: TUBE LENGTH
00056   C     2: TUBE DIAMETER
00057   C     3: X LOC OF TUBE END 1
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00058   C     4: Y LOC OF TUBE END 1
00059   C     5: X LOC OF TUBE END 2
00060   C     6: Y LOC OF TUBE END 2
00061   C     7: X SHIFT IN TUBE POSITION
00062   C     8: Y SHIFT IN TUBE POSITION
00063   C     9: BOUNDARY NUMBER OF TUBE IDT
00064   C    10: FLUID VELOCITY
00065   C    11: MASS FLOW RATE
00066   C    12: TUBE VOLUME
00067   C
00068   C   XNOD (IDN) AND YNOD (IDN)
00069   C     1: X AND Y COORDINATES OF NODE IDN
00070   C
00071   C   IDNOD (L,ID)
00072   C     1: NODE NUMBER ASST WITH SIDE L OF SEED ID
00073   C
00074   C   IDTUB (L,ID)
00075   C     1: TUBE NUMBER OF SIDE L OF SEED ID
00076   C
00077   C   TUBNOD (K,IDT)
00078   C     1: NODE NUMBER AT TUBE END 1
00079   C     2: NODE NUMBER AT TUBE END 2
00080   C     3: SEED NUMBER OF 1ST PARTICLE
00081   C     4: SEED NUMBER OF 2ND PARTICLE
00082   C
00083         PI=4.*ATAN(1.)
00084         TWOPI = 2. *PI
00085         RT3 = SQRT(3.)
00086         RT2 = SQRT(2.)
00087         ISED = 111311
00088         PRINT*,4.*ATAN(1.),4.*ATAN(-1.)
00089   C
00090         CALL TK4014(960,1)
00091         CALL PAGE(11.,8.5)
00092         CALL BLOWUP(5./4.)
00093         CALL NOBRDR
00094         CALL YAXANG(0.)
00095         CALL HEIGHT(0.10)
00096         CALL DUPLX
00097         CALL XREVTK
00098         CALL YREVTK
00099         CALL GAPWID(.002)
00100         CALL THKFRM(.030)
00101         CALL GRACE(2.0)
00102         CALL NOCHEK
00103   C
00104   1600  CONTINUE
00105         ICONT = 0
00106   C
00107         DO 1480 ID=1,500
00108           DO 1480 L=1,12
00109    1480     IDNOD(L,ID)=0
00110   C
00111         DO 1404 IDN=1,1500
00112    1404   NODAR(1,IDN)=0
00113   C
00114         GMIN=0.
```

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```
00115          GMAX=0.
00116          GAVE=0.
00117          CMIN=1.
00118          CMAX=0.
00119    C
00120    1519  CONTINUE
00121          IPROB=1
00122          IF (IPROB.EQ.4) THEN
00123            RBORE=0.1
00124            PRINT*,'INPUT BORE RADIUS',RBORE
00125            READ*,RBORE
00126          ENDIF
00127          IMETH = 4
00128          IFILL = 0
00129          PRINT*,'INPUT IMETH,IFILL',IMETH,IFILL
00130          READ*,IMETH,IFILL
00131          XMAX=1.
00132          YMAX=1.
00133          PRINT*,'INPUT XMAX,YMAX',XMAX,YMAX
00134          READ*,XMAX,YMAX
00135          IDBIN = 4
00136          PRINT*,'INPUT INFLOW BOUNDARY ID',IDBIN
00137          READ*,IDBIN
00138          IDBEV = (IDBIN /2) *2
00139          IDBOU = MOD (IDBIN+1, 4) + 1
00140          IPLTS = 0
00141          IPLTB = 0
00142          IPLTC = 0
00143          PRINT*,'INPUT IPLTC,IPLTS,IPLTB',IPLTC,IPLTS,IPLTB
00144          READ*,IPLTC,IPLTS,IPLTB
00145          IPLTP = 0
00146          IPLTT = 0
00147          IPLTN = 0
00148          ISHAD = 0
00149          PRINT*,'INPUT IPLTP,IPLTT,IPLTN,ISHAD',IPLTP,IPLTT,IPLTN,ISHAD
00150          READ*,IPLTP,IPLTT,IPLTN,ISHAD
00151          IROTA = 0
00152          PRINT*,'ROTATE SEEDS PI/2 ?   0 = NO  1 = YES',IROTA
00153          READ*,IROTA
00154          DEMAX0=3.
00155          PRINT*,'INPUT DEMAX0',DEMAX0
00156          READ*,DEMAX0
00157          NBOX=4
00158    C
00159    C---  INITIALIZE SEED  ---
00160    C
00161          IF (IMETH .LT. 0) THEN
00162    C
00163            REWIND(-IMETH)
00164            READ(-IMETH,*) NSEED,ISEED0,XMAX,YMAX,PORO,SPAC,SPACM,TOL
00165            DO 413 I = 1, NSEED
00166     413      READ(-IMETH,*) XS(I),YS(I),HITE(I),DIAM(I),RADI(I)
00167            READ(-IMETH,*) JNOD
00168            DO 441 IDN = 1, JNOD
00169              READ(-IMETH,*) PRES(IDN)
00170     441      PRESO(IDN) = PRES(IDN)
00171            DIAMF = DIAM(1)
```

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```
00172           PRINT*,'INPUT EPS0,DIAMF',EPS0,DIAMF
00173           READ*,EPS0,DIAMF
00174   C
00175    417    DELDIA = 0.
00176           IREDU = 1
00177           PRINT*,'INPUT IREDU,DELDIA',IREDU,DELDIA
00178           READ*,IREDU,DELDIA
00179           SWELL = 0.
00180           PRINT*,'INPUT SWELLING FRACTION',SWELL
00181           READ*,SWELL
00182           IOK=0
00183           PRINT*,'INPUT OK:  0 = NO  1 = YES',IOK
00184           READ*,IOK
00185           IF (IOK .EQ. 0) GO TO 1519
00186   C
00187         ELSEIF (IMETH .EQ. 99) THEN
00188           READ(99,*) NPAR,XMAX,YMAX,EPS0,DIAMF
00189           DO 693 ID = 1,NPAR
00190             READ(99,*) XS(ID),YS(ID),HITE(ID),DIAM(ID),RADI(ID)
00191    693    CONTINUE
00192
00193         ELSEIF (IMETH .EQ. 1) THEN
00194           FAC=1
00195           NSEED=150
00196           PRINT*,'INPUT NSEED,ISED',NSEED,ISED
00197           READ*,NSEED,ISED
00198           ISEED0=ISED
00199           DSAT=1.
00200           PRINT*,'INPUT DSAT',DSAT
00201           READ*,DSAT
00202           DSMIN=ABS(DSAT)*0.80/SQRT(1.*NSEED)
00203           DREF = DSMIN
00204           POROIN=.4
00205           ALOGSIG = 1.E-8
00206           PRINT*,'INPUT PORO,SIG',POROIN,ALOGSIG
00207           READ*,POROIN,ALOGSIG
00208           DELDIA = 0.
00209           IREDU = 1
00210           PRINT*,'INPUT IREDU,DELDIA',IREDU,DELDIA
00211           READ*,IREDU,DELDIA
00212           SWELL = 0.
00213           PRINT*,'INPUT SWELLING FRACTION',SWELL
00214           READ*,SWELL
00215           IOK=0
00216           PRINT*,'INPUT OK:  0 = NO  1 = YES',IOK
00217           READ*,IOK
00218           IF (IOK.EQ.0) GO TO 1519
00219   C
00220           KSEED=0
00221           SUMP=0.
00222           NBSUM=0
00223           IF (DSAT.EQ.1) NSEED=50*NSEED
00224           DO 1010 I=1,NSEED
00225             IDEC(I)=0
00226             ITRY=0
00227             DONE(I)=0
00228             ALOGMU=ALOG(DSMIN/2.)

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```
00229              ZZZ=RAN(ISED)
00230              CALL ERRINV(ALOGR)
00231              DIAM(I)=2.*EXP(ALOGR)
00232    C
00233     1013     XS(I)=XMAX*RAN(ISED)
00234              YS(I)=YMAX*RAN(ISED)
00235              HITE(I)=DIAM(I)/2. *(1.-2.*RAN(ISED))
00236              HMINN = MAX (HITE(I), DSMIN/50.)
00237              IF (HITE(I) .LT. 0.) THEN
00238                HITE(I) = MIN (HITE(I), -HMINN)
00239              ELSE
00240                HITE(I) = MAX (HITE(I), HMINN)
00241              ENDIF
00242              RADI(I)=SQRT( (DIAM(I)/2.)**2 - HITE(I)**2 )
00243    C
00244              IF (DSAT.GT.1.E-6) THEN
00245                RPART=RADI(I)
00246                DELBO=RPART-XS(I)
00247                DELBO=MAX(DELBO,XS(I)+RPART-XMAX)
00248                DELBO=MAX(DELBO,RPART-YS(I))
00249                DELBO=MAX(DELBO,YS(I)+RPART-YMAX)
00250                IF ( DELBO.GT.0.0) THEN
00251                  ITRY=ITRY+1
00252                  IF (ITRY.GT.MAX(100,200*KSEED)) GO TO 1014
00253                  GO TO 1013
00254                ENDIF
00255                EPSR2 = (DSMIN /100.)**2
00256                DO 1012 J=1,I-1
00257                  DELX2=(XS(I)-XS(J))**2
00258                  DELY2=(YS(I)-YS(J))**2
00259                  DELH2=(HITE(I)-HITE(J))**2
00260                  DELR2=((DIAM(I)+DIAM(J))/2.)**2
00261                  IF ( DELX2+DELY2+DELH2.LT.DELR2+EPS2 ) THEN
00262                    ITRY=ITRY+1
00263                    IF (ITRY.GT.MAX(100,200*KSEED)) GO TO 1014
00264                    GO TO 1013
00265                  ENDIF
00266     1012       CONTINUE
00267              ENDIF
00268    C
00269              SUMP=SUMP+3.14*RADI(I)**2
00270              PORO=1.-SUMP/(XMAX*YMAX)
00271              IF (PORO.LT.POROIN) GO TO 1014
00272
00273     1016     KSEED=KSEED+1
00274     1010   CONTINUE
00275     1014   NSEED=KSEED
00276    C
00277          ELSEIF (IMETH.EQ.2) THEN
00278            NSEED = 150
00279            PRINT*,'INPUT NSEED,ISED',NSEED,ISED
00280            READ*,NSEED,ISED
00281            ISEED0 = ISED
00282            DSMIN = SQRT(XMAX*YMAX) *0.80/SQRT(1.*NSEED)
00283            DREF = DSMIN
00284            ALOGSIG = 1.E-8
00285            PRINT*,'INPUT SIG',ALOGSIG

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00286            READ*,ALOGSIG
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```
00287           DELDIA = 0.
00288           IREDU = 1
00289           PRINT*,'INPUT IREDU,DELDIA',IREDU,DELDIA
00290           READ*,IREDU,DELDIA
00291           SWELL = 0.
00292           PRINT*,'INPUT SWELLING FRACTION',SWELL
00293           READ*,SWELL
00294           IOK=0
00295           PRINT*,'INPUT OK:  0 = NO  1 = YES',IOK
00296           READ*,IOK
00297           IF (IOK.EQ.0) GO TO 1519
00298    C
00299           KSEED=0
00300           SUMP=0.
00301           NBSUM=0
00302           NSEED = 10 *NSEED
00303           NDIVX = 20 *XMAX /DSMIN
00304           NDIVY = 20 *YMAX /DSMIN
00305           NDIV = MAX (NDIVX, NDIVY)
00306           NACROS = XMAX /DSMIN
00307           EPS = 1.1 *XMAX /(NDIVX+1.)
00308           PRINT*,NDIVX,NDIVY,EPS
00309           YTOP = 0.
00310           DO 2010 I = 1,NSEED
00311             IDBC(I) = 0
00312             DONE(I) = 0
00313    C
00314             ALOGMU=ALOG(DSMIN/2.)
00315             ZZZ=RAN(ISED)
00316             CALL ERRINV(ALOGR)
00317             DIAM(I)=2.*EXP(ALOGR)
00318    C
00319             HITE(I)=DIAM(I)/2. *(1.-2.*RAN(ISED))
00320             RADI(I)=SQRT( (DIAM(I)/2.)**2 - HITE(I)**2 )
00321             BOTF = 2.* RAN(ISED)
00322    C
00323             YMIN = YMAX
00324             RPART = IFILL *RADI(I)
00325             DO 2022 II = 1,NDIVX
00326               XST = (XMAX *II) /(NDIVX+1.)
00327               DELBO = XST - RPART
00328               DELBO = MIN (DELBO,XMAX-XST-RPART)
00329               IF (DELBO .LT. EPS) GO TO 2022
00330               DO 2023 JJ = 1,NDIVY
00331                 YST = YMAX *(1.- (1.*JJ)/(NDIVY+1.))
00332                 IF (YST .GT. YTOP+DEMAX0*DSMIN) GO TO 2023
00333                 DELBO = YST - RPART
00334                 IF (IFILL .EQ. 0) DELBO = YST - RADI(I) *BOTF
00335                 IF ( DELBO .LT. EPS) THEN
00336                   YMIN = YST
00337                   XS(I) = XST + 1.E-2 *RADI(I)
00338                   YS(I) = YST + 1.E-2 *RADI(I)
00339                   GO TO 2022
00340                 ENDIF
00341                 JJJJMX = MIN (I-1, 4 *NACROS)
00342                 DO 2012 JJJJ = 1,JJJJMX

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00343                   J = I-1 - JJJJ + 1
00344                   DELX2 = (XST-XS(J))**2
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00345                   DELY2 = (YST-YS(J))**2
00346                   DELH2 = (HITE(I)-HITE(J))**2
00347                   DELR2 = ((DIAM(I)+DIAM(J))/2.)**2
00348                   DIST = SQRT (DELX2+DELY2+DELH2) - SQRT (DELR2)
00349                   IF (DIST .LT. EPS) THEN
00350                     IF (YST .LT. YMIN) THEN
00351                       YMIN = YST
00352                       XS(I) = XST + 1.E-2 *RADI(I)
00353                       YS(I) = YST + 1.E-2 *RADI(I)
00354                     ENDIF
00355                     GO TO 2022
00356                   ENDIF
00357    2012         CONTINUE
00358    2023       CONTINUE
00359    2022     CONTINUE
00360             YTOP = YS(I)
00361    C
00362             PRINT1901,I,XS(I),YS(I),RADI(I)
00363             DELBO = YMAX-YS(I)-RPART
00364             IF (DELBO .LT. EPS) GO TO 2014
00365             KSEED = KSEED + 1
00366             SUMP = SUMP + PI *RADI(I)**2
00367             PORO = 1.-SUMP/(XMAX*YMAX)
00368    C
00369     2010   CONTINUE
00370     2014   NSEED = KSEED
00371            PRINT*,NSEED
00372            PRINT*,PORO
00373            READ*, DDXX
00374    C
00375          ELSEIF (IMETH.EQ.5) THEN
00376            NSEED = 150
00377            PRINT*,'INPUT ISED',ISED
00378            READ*,ISED
00379            ISEED0 = ISED
00380            PRINT*,'INPUT FIBER DIAM AND POROISTY',DIAMF,EPS0
00381            READ*,DIAMF,EPS0
00382            IRAG = 1
00383            PRINT*,'DO YOU WANT A RAGGED BOTTOM:  0 = NO    1 = YES',IRAG
00384            READ*,IRAG
00385            DSMIN = DIAMF
00386            DREF = DSMIN
00387            DELDIA = 0.
00388            IREDU = 1
00389            PRINT*,'INPUT IREDU,DELDIA',IREDU,DELDIA
00390            READ*,IREDU,DELDIA
00391            SWELL = 0.
00392            PRINT*,'INPUT SWELLING FRACTION',SWELL
00393            READ*,SWELL
00394            IOK=0
00395            ACON = 1
00396            PRINT*,'INPUT RANDOM VARIATION IN SPACING ( 0 TO 1) ',ACON
00397            READ*,ACON
00398            PRINT*,'INPUT OK:  0 = NO  1 = YES',IOK
00399            READ*,IOK

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00400            IF (IOK.EQ.0) GO TO 1519
00401    C
00402            KSEED=0
```

```
00403           SUMP=0.
00404           NBSUM=0
00405           NSEED = 2 * XMAX *YMAX / (PI/4. *DIAMF**2) *(1.-EPS0)
00406           NDIVX = 20 *XMAX /DIAMF
00407           NDIVY = 20 *YMAX /DIAMF
00408           NDIV = MAX (NDIVX, NDIVY)
00409           NACROS = XMAX /DSMIN
00410           TOL = 1.1 *XMAX /(NDIVX+1.)
00411           RHO = 1. - EPS0
00412           DSMIN = DIAMF /SQRT(2.*RT3/PI*RHO)
00413           PRINT*,NDIVX,NDIVY,TOL
00414           YTOP = 0.
00415           DO 5010 I = 1,NSEED
00416             IDBC(I) = 0
00417             DONE(I) = 0
00418   C
00419             DIAM(I)=DIAMF
00420   C
00421             HITE(I)=0.
00422             RADI(I)=SQRT( (DIAM(I)/2.)**2 - HITE(I)**2 )
00423             BOTF = 2.* RAN(ISED)
00424             SPAC = (1. + ACON*(1.-BOTF)) *(DSMIN - DIAMF)
00425             SPAC = MAX (0., SPAC)
00426             SPACM = SPAC + TOL
00427             RANX = (1. - BOTF) *SPACM /100.
00428             RANY = (1. - 2.*RAN(ISED)) *SPACM /100.
00429   C
00430             YMIN = YMAX
00431             JMIN1 = 0
00432             RPART = IFILL *RADI(I)
00433             DO 5022 II = 1,NDIVX
00434               XST = (XMAX *II) /(NDIVX+1.)
00435               DELBO = XST - RPART
00436               DELBO = MIN (DELBO,XMAX-XST-RPART)
00437               IF (DELBO .LT. TOL) GO TO 5022
00438               DO 5023 JJ = 1,NDIVY
00439                 YST1 = YMAX *(1.- (1.*JJ)/(NDIVY+1.))
00440                 NUMY = (YTOP+DSMIN+SPACM) *(NDIVY+1.) /YMAX + 1
00441                 YST2 = YMAX *(NUMY-JJ+1.) /(NDIVY+1.)
00442                 YST = MIN (YST1, YST2)
00443                 DELBO = YST - RPART
00444                 IF (IFILL .EQ. 0) DELBO = YST - RADI(I) *IRAG *BOTF
00445                 IF ( DELBO .LT. TOL) THEN
00446                   JJY = JJ
00447                   YMIN = YST
00448                   XS(I) = XST + RANX
00449                   YS(I) = YST + RANY
00450                   GO TO 5022
00451                 ENDIF
00452                 JJJJMX = MIN (I-1, 2 *NACROS)
00453                 DO 5012 JJJJ = 1,JJJJMX
00454                   J = I-1 - JJJJ + 1
00455                   DELX2 = (XST-XS(J))**2
00456                   DELY2 = (YST-YS(J))**2

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00457                   DELH2 = (HITE(I)-HITE(J))**2
00458                   DELR2 = ((DIAM(I)+DIAM(J))/2.)**2
00459                   DIST = SQRT (DELX2+DELY2+DELH2) - SQRT (DELR2)
00460                   IF (DIST .LT. SPACM) THEN
```

```
00461                     IF (YST .LT. YMIN) THEN
00462                       JJY = JJ
00463                       YMIN = YST
00464                       XS(I) = XST + RANX
00465                       YS(I) = YST + RANY
00466                       SPAC1 = DIST
00467                       JMIN1 = J
00468                     ENDIF
00469                     GO TO 5022
00470                   ENDIF
00471    5012         CONTINUE
00472    5023       CONTINUE
00473    5022     CONTINUE
00474   C
00475   C---  FIND SECOND CLOSEST PARTICLE BELOW ---
00476   C
00477             SMIN = YMAX
00478             JMIN2 = 0
00479             DO 5044 J = 1, I-1
00480               IF (J .EQ. JMIN1) GO TO 5044
00481               IF (YS(I)-YS(J) .LT. 3.*TOL .AND. JMIN1.GT.0) GO TO 5044
00482               DELX2 = (XS(I)-XS(J))**2
00483               DELY2 = (YS(I)-YS(J))**2
00484               DELH2 = (HITE(I)-HITE(J))**2
00485               DELR2 = ((DIAM(I)+DIAM(J))/2.)**2
00486               DIST = SQRT (DELX2+DELY2+DELH2) - SQRT (DELR2)
00487               IF (DIST .GT. DIAM(I)/3.) GO TO 5044
00488               IF (DIST .LT. SMIN) THEN
00489                 SMIN = DIST
00490                 JMIN2 = J
00491               ENDIF
00492    5044     CONTINUE
00493             SPAC2 = SMIN
00494   C
00495   C---  MOVE FIBER TO EQUILIBRIUM POSITION
00496   C
00497             BCON = TOL /10.
00498   C
00499             IF (JMIN1.EQ.0 .AND. JMIN2.EQ.0) THEN
00500               CC1 = 0.
00501               CC2 = 0.
00502               AA1 = 1.
00503               AA2 = 0.
00504               BB1 = 0.
00505               BB2 = 1.
00506
00507             ELSEIF (JMIN1.EQ.0 .AND. JMIN2.GT.0) THEN
00508               CC1 = (DIAM(I)/2. + DIAM(JMIN2)/2. + SPAC + BCON)**2
00509        1            - (XS(I)-XS(JMIN2))**2 - (YS(I)-YS(JMIN2))**2
00510               CC2 = 0.
00511               AA1 = 2. *(XS(I)-XS(JMIN2))
00512               AA2 =    YS(I)-YS(JMIN2)
00513               BB1 = 2. *(YS(I)-YS(JMIN2))

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00514               BB2 = - (XS(I)-XS(JMIN2))
00515   C
00516             ELSEIF (JMIN1.GT.0 .AND. JMIN2.EQ.0) THEN
00517               CC1 = (DIAM(I)/2. + DIAM(JMIN1)/2. + SPAC + BCON)**2
00518        1            - (XS(I)-XS(JMIN1))**2 - (YS(I)-YS(JMIN1))**2
```

```
00519              CC2 = 0.
00520              AA1 = 2. *(XS(I)-XS(JMIN1))
00521              AA2 =    YS(I)-YS(JMIN1)
00522              BB1 = 2. *(YS(I)-YS(JMIN1))
00523              BB2 = - (XS(I)-XS(JMIN1))
00524   C
00525            ELSEIF (JMIN1.GT.0 .AND. JMIN2.GT.0) THEN
00526              CC1 = (DIAM(I)/2. + DIAM(JMIN1)/2. + SPAC + BCON)**2
00527        1           - (XS(I)-XS(JMIN1))**2 - (YS(I)-YS(JMIN1))**2
00528              CC2 = (DIAM(I)/2. + DIAM(JMIN2)/2. + SPAC + BCON)**2
00529        1           - (XS(I)-XS(JMIN2))**2 - (YS(I)-YS(JMIN2))**2
00530              AA1 = 2. *(XS(I)-XS(JMIN1))
00531              AA2 = 2. *(XS(I)-XS(JMIN2))
00532              BB1 = 2. *(YS(I)-YS(JMIN1))
00533              BB2 = 2. *(YS(I)-YS(JMIN2))
00534            ENDIF
00535            DLTX = (CC1*BB2-CC2*BB1) /(AA1*BB2-AA2*BB1)
00536            DLTY = (CC2 - AA2*DLTX) /BB2
00537            RLIM = (2.*TOL)**2
00538            IF (DLTX**2+DLTY**2 .GT. RLIM) THEN
00539              DLTX = 0.
00540              DLTY = 0.
00541            ENDIF
00542            XS(I) = XS(I) + DLTX
00543            YS(I) = YS(I) + DLTY
00544   C
00545            XS(I) = MAX (XS(I),TOL+RANX)
00546            XS(I) = MIN (XS(I), XMAX-TOL-RANX)
00547            YS(I) = MAX (YS(I), TOL+RANY)
00548            YS(I) = MIN (YS(I), YMAX-TOL-RANY)
00549   C
00550            YTOP = MAX (YS(I), YTOP)
00551   C
00552            DELBO = YMAX-YS(I)-RPART
00553            IF (DELBO .LT. TOL) GO TO 5014
00554            IF (JJY .EQ. 1) GO TO 5014
00555            PRINT1903,I,JMIN1,JMIN2,XS(I),YS(I),RADI(I),SPAC,DLTX,DLTY
00556            KSEED = KSEED + 1
00557            SUMP = SUMP + PI *RADI(I)**2
00558            PORO = 1.-SUMP/(XMAX*YMAX)
00559   C
00560    5010   CONTINUE
00561    5014   NSEED = KSEED
00562           PRINT*,NSEED
00563           PRINT*,PORO
00564           READ*, DDXX
00565   C
00566         ELSEIF (IMETH.EQ.3) THEN
00567           NSEED = 150
00568           PRINT*,'INPUT NSEED,ISED',NSEED,ISED
00569           READ*,NSEED,ISED
00570           ISEED0 = ISED

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00571           DSMIN = SQRT(XMAX*YMAX) *0.80/SQRT(1.*NSEED)
00572           DREF = DSMIN
00573           ALOGSIG = 1.E-8
00574           PRINT*,'INPUT SIG',ALOGSIG
00575           READ*,ALOGSIG
00576           DELDIA = 0.
```

```
00577           IREDU = 1
00578           PRINT*,'INPUT IREDU,DELDIA',IREDU,DELDIA
00579           READ*,IREDU,DELDIA
00580           SWELL = 0.
00581           PRINT*,'INPUT SWELLING FRACTION',SWELL
00582           READ*,SWELL
00583           IOK=0
00584           PRINT*,'INPUT OK:  0 = NO  1 = YES',IOK
00585           READ*,IOK
00586           IF (IOK.EQ.0) GO TO 1519
00587   C
00588           KSEED=0
00589           SUMP=0.
00590           NBSUM=0
00591           NSEED = 10 *NSEED
00592           NDIVX = 10 *XMAX /DSMIN
00593           NDIVY = 10 *YMAX /DSMIN
00594           NDIVZ = 10
00595           NDIV = MAX (NDIVX, NDIVY)
00596           NACROS = XMAX /DSMIN
00597           EPS = 1.1 *XMAX /(NDIVX+1.)
00598           PRINT*,NDIVX,NDIVY,EPS
00599           YTOP = 0.
00600           DO 3010 I = 1,NSEED
00601             IDBC(I) = 0
00602             DONE(I) = 0
00603   C
00604             ALOGMU=ALOG(DSMIN/2.)
00605             ZZZ=RAN(ISED)
00606             CALL ERRINV(ALOGR)
00607             DIAM(I)=2.*EXP(ALOGR)
00608             BOTF = 2.* RAN(ISED)
00609   C
00610             YMIN = YMAX
00611             DO 3022 II = 1,NDIVX
00612               XST = (XMAX *II) /(NDIVX+1.)
00613               DELBO = XST - RPART
00614               DELBO = MIN (DELBO,XMAX-XST-RPART)
00615               IF (DELBO .LT. EPS) GO TO 3022
00616               DO 3021 KK = 1,NDIVZ
00617                 HIT = DIAM(I)/2. *(1.- 2.*(1.*KK)/(NDIVZ+1.))
00618                 IF (I.LT.NACROS) HIT = DIAM(I)/2. *(1.-2.*RAN(ISED))
00619                 RAD = SQRT( (DIAM(I)/2.)**2 - HIT**2 )
00620                 RPART = IFILL *RAD
00621                 DO 3023 JJ = 1,NDIVY
00622                   YST = YMAX *(1.- (1.*JJ)/(NDIVY+1.))
00623                   IF (YST .GT. YTOP+DEMAX0*DSMIN) GO TO 3023
00624                   DELBO = YST - RPART
00625                   IF (IFILL .EQ. 0) DELBO = YST - RAD *BOTF
00626                   IF ( DELBO .LT. EPS) THEN
00627                     YMIN = YST

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00628                     XS(I) = XST + 1.E-2 *RAD
00629                     YS(I) = YST + 1.E-2 *RAD
00630                     HITE(I) = HIT
00631                     RADI(I) = RAD
00632                     GO TO 3022
00633                   ENDIF
00634                   JJJJMX = MIN (I-1, 3 *NACROS)
```

```
00635                   DO 3012 JJJJ = 1,JJJJMX
00636                     J = I-1 - JJJJ + 1
00637                     DELX2 = (XST-XS(J))**2
00638                     DELY2 = (YST-YS(J))**2
00639                     DELH2 = (HIT-HITE(J))**2
00640                     DELR2 = ((DIAM(I)+DIAM(J))/2.)**2
00641                     DIST = SQRT (DELX2+DELY2+DELH2) - SQRT (DELR2)
00642                     IF (DIST .LT. EPS) THEN
00643                       IF (YST .LT. YMIN) THEN
00644                         YMIN = YST
00645                         RADI(I) = RAD
00646                         XS(I) = XST + 1.E-2 *RADI(I)
00647                         YS(I) = YST + 1.E-2 *RADI(I)
00648                         HITE(I) = HIT
00649                       ENDIF
00650                       GO TO 3021
00651                     ENDIF
00652    3012           CONTINUE
00653    3023         CONTINUE
00654    3021       CONTINUE
00655    3022     CONTINUE
00656             YTOP = YS(I)
00657   C
00658             PRINT1901,I,XS(I),YS(I),2.*HITE(I)/DIAM(I),RADI(I)
00659             DELBO = YMAX-YS(I)-RPART
00660             IF (DELBO .LT. EPS) GO TO 3014
00661             KSEED = KSEED + 1
00662             SUMP = SUMP + PI *RADI(I)**2
00663             PORO = 1.-SUMP/(XMAX*YMAX)
00664   C
00665    3010   CONTINUE
00666    3014   NSEED = KSEED
00667           PRINT*,NSEED
00668           PRINT*,PORO
00669           READ*,DDXX
00670   C
00671         ELSEIF (IMETH.EQ.4) THEN
00672           IPAK = 1
00673           PRINT*,'INPUT IPAK:  1 = HEX    2 = STAGGERED',IPAK
00674           READ*,IPAK
00675           EPS0 = 0.3
00676           DIAMF = 0.1
00677           PRINT*,'INPUT FIBER DIAMETER AND POROISTY',DIAMF,EPS0
00678           READ*,DIAMF,EPS0
00679           DREF = DIAMF
00680           DELDIA = 0.
00681           IREDU = 1
00682           PRINT*,'INPUT IREDU,DELDIA',IREDU,DELDIA
00683           READ*,IREDU,DELDIA
00684           ACON = 0

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00685           PRINT*,'INPUT RANDOM VARIATION IN SPACING ( 0 TO 1) ',ACON
00686           READ*,ACON
00687           ISED = 12344321
00688           PRINT*,'INPUT SEED FOR RANDOM DISPLACEMENT',ISED
00689           READ*,ISED
00690   C
00691           RHOS = 1. - EPS0
00692           DXXX = DIAMF *SQRT(PI /2. /RT3 /RHOS)
```

```
00693           IF (IPAK .EQ. 2) DXXX = DIAMF *SQRT(PI /2. /RHOS)
00694           NX = NINT (XMAX /DXXX) + 1
00695           XMAX = (NX-1) *DXXX
00696           DYDX = RT3
00697           IF (IPAK .EQ. 2) DYDX = 1.
00698           FAC = DYDX /2.
00699           DYYY = FAC *DXXX
00700           NY = NINT (YMAX /DYYY) + 1
00701           YMAX = (NY-1) *DYYY
00702           SPAC = DXXX - DIAMF
00703           IF (IPAK .EQ. 2) SPAC = DXXX /RT2 - DIAMF
00704           SPAC0 = SPAC
00705           DISD = 0.000 *50.
00706           PRINT*,'INPUT FACTOR FOR RANDOMIZATION',DISD
00707           READ*,DISD
00708           IPLTWK = 0
00709           IF (DISD .GT. 0.) THEN
00710             PRINT*,'PLOT RANDOM MOTION ?  0 = NO  1 = YES',IPLTWK
00711             READ*,IPLTWK
00712           ENDIF
00713           SWELL = 0.
00714           PRINT*,'INPUT SWELLING FRACTION',SWELL
00715           READ*,SWELL
00716           IOK=0
00717           PRINT*,'INPUT OK:  0 = NO  1 = YES',IOK
00718           READ*,IOK
00719           IF (IOK.EQ.0) GO TO 1519
00720   C
00721           KSEED = 0
00722           EPS = 1.E-3 *SQRT(XMAX*YMAX)
00723           EPS = MIN (EPS, SPAC/100.)
00724           ID = 0
00725           DO 1025 I=1,NY
00726             JD=1-MOD(I,2)
00727             DO 1015 J=1,NX-JD
00728               ID = ID + 1
00729               THET = 2.*PI *RAN(ISED)
00730               DELS = SPAC *(0.5-RAN(ISED))
00731               XS(ID)=(J-1)*DXXX+JD*DXXX/2. + ACON *DELS *COS(THET)
00732               YS(ID)=DYYY*(I-1) + ACON *DELS *SIN(THET)
00733               HITE(ID) = 0.
00734               DIAM(ID) = DIAMF
00735               RADI(ID) = DIAMF /2.
00736               DBOX(ID) = EPS
00737               WORK(1,ID) = XS(ID)
00738               WORK(2,ID) = YS(ID)
00739   C
00740   1015      CONTINUE
00741   1025    CONTINUE

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00742           KSEED = ID
00743           NSEED = KSEED
00744           NPAR = NSEED
00745         ENDIF
00746   C
00747   C---  ROUGH POROSITY, SPAC, ETC.  ---
00748   C
00749         NPAR = NSEED
00750         VSUM = 0.
```

```
00751         RBAR = 0.
00752         DBAR = 0.
00753         DO 887 ID = 1, NPAR
00754           RBAR = RBAR + RADI(ID)
00755           DBAR = DBAR + DIAM(ID)
00756           ARID = PI * RADI(ID)**2
00757           VSUM = VSUM + ARID
00758    887  CONTINUE
00759         RBAR = RBAR /NPAR
00760         DBAR = DBAR /NPAR
00761         PORO = 1. - VSUM /(XMAX*YMAX)
00762         RHOS = 1. - PORO
00763         HLEG = SQRT (PI /2. /RT3 /RHOS) *DBAR
00764         SPAC = HLEG - DBAR
00765         SPAC = MAX (SPAC, DBAR /100.)
00766         DIAMF = DBAR
00767         DREF = DBAR
00768   C
00769   C---  RANDOMIZE SEED LOCATIONS  ---
00770   C
00771           DISD = 0.000 *50.
00772           PRINT*,'INPUT FACTOR FOR RANDOMIZATION',DISD
00773           READ*,DISD
00774           IPLTWK = 0
00775           IF (DISD .GT. 0.) THEN
00776             PRINT*,'PLOT RANDOM MOTION ?  0 = NO  1 = YES',IPLTWK
00777             READ*,IPLTWK
00778           ENDIF
00779    1784   NBORS = 6
00780           NDARR = 18
00781           CALL NERNEB (NDARR,NBORS,NSEED,XS,YS,X0,Y0,DNEIGH,INEIGH)
00782           DELS = SPAC /10.
00783           DELS0 = DELS
00784           KCYMX = DISD *DIAMF /DELS
00785           IF (KCYMX .GT. 0) THEN
00786             IF (IPLTWK .EQ. 1) THEN
00787               XORIG = 0.
00788               YORIG = 0.
00789               RATXY = XMAX /YMAX
00790               IF (RATXY.GT.1.0) THEN
00791                 XAXIS = 7.5
00792                 YAXIS=XAXIS *0.95775 /RATXY
00793               ELSE
00794                 XAXIS = 7.5 *RATXY
00795                 YAXIS=XAXIS *0.95775 /RATXY
00796               ENDIF
00797               XSTP = (XMAX - XORIG) /1.
00798               YSTP = (YMAX - YORIG) /1.

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00799               CALL AREA2D(XAXIS,YAXIS)
00800               CALL GRAF(XORIG,XSTP,XMAX,YORIG,YSTP,YMAX)
00801               CALL FRAME
00802               CALL MARKER(15)
00803               CALL CURVE(XS,YS,NSEED,-1)
00804             ENDIF
00805   C
00806             SLMAX = 0.
00807             ITRYMX = 100
00808             DO 1091 KCY = 1, KCYMX
```

```
00809                JMOV = 0
00810                DO 1092 I = 1, NSEED
00811                  ITRY = 0
00812                  DELS = DELS0
00813     651          THET = 2. * PI *RAN(ISED)
00814                  DELX = DELS *COS(THET)
00815                  DELY = DELS *SIN(THET)
00816                  XNEW = XS(I) + DELX
00817                  YNEW = YS(I) + DELY
00818                  TOL = DBOX(I)
00819                  IF (XNEW .LT. TOL) XNEW = 2.*TOL - XNEW
00820                  IF (XNEW .GT. XMAX-TOL) XNEW = 2.*(XMAX-TOL) - XNEW
00821                  IF (YNEW .LT. TOL) YNEW = 2.*TOL - YNEW
00822                  IF (YNEW .GT. YMAX-TOL) YNEW = 2.*(YMAX-TOL) - YNEW
00823                  DO 1093 JJ = 1, NBORS
00824                    J = INEIGH(JJ,I)
00825                    DIST = SQRT((XNEW-XS(J))**2 + (YNEW-YS(J))**2)
00826                    IF (DIST .LT. RADI(I)+RADI(J)) THEN
00827                      IF (ITRY .GT. ITRYMX) GO TO 1092
00828                      ITRY = ITRY + 1
00829                      GO TO 651
00830                    ENDIF
00831     1093         CONTINUE
00832                  JMOV = JMOV + 1
00833                  XS(I) = XNEW
00834                  YS(I) = YNEW
00835                  SL(I) = SQRT ((XS(I)-X0(I))**2 + (YS(I)-Y0(I))**2)
00836                  SLMAX = MAX (SL(I), SLMAX)
00837     1092       CONTINUE
00838    C
00839                IF (MOD(KCY-1, MAX(1,KCYMX/500)) .EQ. 0) THEN
00840                  CALL SPACEF (57,NSEED,XS,YS,XMAX,YMAX,SDEVX,SDEVY)
00841                  WRITE(16,900) KCY*DELS/DIAMF,SDEVX,SDEVY
00842                ENDIF
00843    C
00844                IF (SLMAX .GT. DIAMF/3.) THEN
00845                  DISMX = 0.
00846                  DISBR = 0
00847                  DISX  = 0.
00848                  DISY  = 0.
00849                  DO 1855 ID = 1, NSEED
00850                    DSID = (XS(ID)-WORK(1,ID))**2 + (YS(ID)-WORK(2,ID))**2
00851                    DSID = SQRT (DSID)
00852                    DISMX = MAX (DISMX, DSID)
00853                    DISBR = DISBR + DSID
00854                    DISX = MAX (DISX, ABS(XS(ID)-WORK(1,ID)))
00855                    DISY = MAX (DISY, ABS(YS(ID)-WORK(2,ID)))

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00856                    IF (IPLTWK .EQ. 1) THEN
00857                      XB(1) = X0(ID)
00858                      XB(2) = XS(ID)
00859                      YB(1) = Y0(ID)
00860                      YB(2) = YS(ID)
00861                      CALL CURVE(XB,YB,2,0)
00862                    ENDIF
00863     1855         CONTINUE
00864                  DISBR = DISBR /NSEED
00865                  CALL SPACEF (87,NSEED,XS,YS,XMAX,YMAX,SDEVX,SDEVY)
00866                  WRITE(17,900) KCY*DELS/DIAMF,DISMX/DIAMF,DISBR/DIAMF,
```

```
00867       1                    SDEVX,SDEVY,DISMX/SPAC,DISBR/SPAC
00868   C
00869                SLMAX = 0.
00870                CALL NERNEB (NDARR,NBORS,NSEED,XS,YS,X0,Y0,DNEIGH,INEIGH)
00871   C
00872                IF (IPLTWK .EQ.0) THEN
00873                  CBAR = 0
00874                  NSUM = 0
00875                  DO 1101 ID = 1, NSEED
00876                    DBXX = MIN (XS(ID), XMAX-XS(ID)) /DIAMF
00877                    DBXY = MIN (YS(ID), YMAX-YS(ID)) /DIAMF
00878                    IF (DBXX.LT.2.0 .OR. DBXY.LT.2.0) GO TO 1101
00879                    DO 1101 J = 1, NBORS
00880                      NSUM = NSUM + 1
00881                      CBAR = CBAR + DNEIGH(J,ID)
00882    1101            CONTINUE
00883                  CBAR = CBAR /NSUM
00884                  SDEV = 0.
00885                  DO 1102 ID = 1, NSEED
00886                    DBXX = MIN (XS(ID), XMAX-XS(ID)) /DIAMF
00887                    DBXY = MIN (YS(ID), YMAX-YS(ID)) /DIAMF
00888                    IF (DBXX.LT.2.0 .OR. DBXY.LT.2.0) GO TO 1102
00889                    DO 1102 J = 1, NBORS
00890                    SDEV = SDEV +(DNEIGH(J,ID)-CBAR)**2
00891    1102            CONTINUE
00892                  SDEV = SQRT (SDEV /(NSUM-1.))
00893                  PRINT901,JMOV,CBAR,SDEV,SDEVX,SDEVY,DISX,DISY
00894                ENDIF
00895              ENDIF
00896    1091    CONTINUE
00897   C
00898              IF (IPLTWK .EQ. 1) CALL ENDPL(0)
00899              ICRAN = 1
00900              PRINT*,'MORE RANDOMIZING ?  0 = NO  1 = YES',ICRAN
00901              READ*,ICRAN
00902              IF (ICRAN .EQ. 1) THEN
00903                CALL SPACEF (87,NSEED,XS,YS,XMAX,YMAX,SDEVX,SDEVY)
00904                PRINT900,SDEX,SDEVY
00905                PRINT*,'INPUT FACTOR FOR RANDOMIZATION',DISD
00906                READ*,DISD
00907                PRINT*,'PLOT RANDOM MOTION ?  0 = NO  1 = YES',IPLTWK
00908                READ*,IPLTWK
00909                GO TO 1784
00910              ENDIF
00911            ENDIF
00912   C

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00913   C---  TAKE SUBSET OF PARTICLES
00914   C
00915          ISUB = 0
00916          PRINT*,'TAKE SUBSET OF PARTICLES ?  0 = NO  1 = YES',ISUB
00917          READ*,ISUB
00918          IF (ISUB .EQ. 1) THEN
00919            X0NEW = 0.
00920            Y0NEW = 0.
00921            XMAXN = XMAX
00922            YMAXN = YMAX
00923            PRINT*,'INPUT XORIG, XMAX, YORIG, YMAX',
00924         1                 X0NEW, XMAXN, Y0NEW, YMAXN
```

```
00925           READ*, X0NEW, XMAXN, Y0NEW, YMAXN
00926           XMAX = XMAXN - X0NEW
00927           YMAX = YMAXN - Y0NEW
00928           DO 519 ID = 1, NSEED
00929             XS(ID) = XS(ID) - X0NEW
00930             YS(ID) = YS(ID) - Y0NEW
00931    519    CONTINUE
00932         ENDIF
00933   C
00934   C---  DROP PARTICLES OUTSIDE BOX FROM SEED SET  ---
00935   C
00936         NSUM = 0
00937         NOUT = 0
00938         SMEAS = SQRT (XMAX*YMAX)
00939         EPS = 1.E-3 *SMEAS
00940         DO 1188 ID = 1, NSEED
00941           DBXX = MIN (XS(ID), XMAX-XS(ID))
00942           DBXY = MIN (YS(ID), YMAX-YS(ID))
00943           DBZZ = MIN (DBXX, DBXY)
00944           IF (DBXX.LT.0.0 .AND. DBXY.LT.0.0) DBZZ = -SQRT(DBXX**2+DBXY**2)
00945           IF (DBZZ .GT. 0.0) THEN
00946             NSUM = NSUM + 1
00947             X0(NSUM) = XS(ID)
00948             Y0(NSUM) = YS(ID)
00949             DIAM0(NSUM) = DIAM(ID)
00950             HITE0(NSUM) = HITE(ID)
00951   C       ELSEIF (DBZZ .GT. EPS-RADI(ID)) THEN
00952           ELSEIF (DBZZ .GT. -0.5 *RADI(ID)) THEN
00953             NOUT = NOUT + 1
00954             WORK(1,NOUT) = XS(ID)
00955             WORK(2,NOUT) = YS(ID)
00956             WORK(3,NOUT) = DIAM(ID)
00957             WORK(4,NOUT) = HITE(ID)
00958           ENDIF
00959    1188 CONTINUE
00960         DO 1189 ID = 1, NSUM
00961           XS(ID) = X0(ID)
00962           YS(ID) = Y0(ID)
00963           DIAM(ID) = DIAM0(ID)
00964           HITE(ID) = HITE0(ID)
00965    1189 CONTINUE
00966         DO 1190 ID = 1, NOUT
00967           XS(ID+NSUM) = WORK(1,ID)
00968           YS(ID+NSUM) = WORK(2,ID)
00969           DIAM(ID+NSUM) = WORK(3,ID)

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00970           HITE(ID+NSUM) = WORK(4,ID)
00971    1190 CONTINUE
00972         NSEED = NSUM + NOUT
00973         NPAR = NSEED
00974   C
00975   C---  ASSIGN RADII AND SWELL PARTICLES  ---
00976   C
00977         DIAMF0 = DIAMF
00978         DIAMF = 0.
00979         DO 1163 ID = 1, NPAR
00980           DIAM0(ID) = DIAM(ID)
00981           DIAM(ID) = DIAM(ID) *(1.+SWELL)
00982           RAD2 = MAX (1.E-20*XMAX, (DIAM(ID)/2.)**2-HITE(ID)**2)
```

```
00983           RADI(ID) = SQRT (RAD2)
00984           DIAMF = DIAMF + DIAM(ID)
00985    1163 CONTINUE
00986         DIAMF = DIAMF /NPAR
00987   C
00988   C---  MONTE CARLO POROSITY  ---
00989   C
00990    491  ISAD = 11554321
00991         NSHOT = 5000
00992         NVOID = 0
00993         DO 492 J = 1, NSHOT
00994           XXX = XMAX *RAN(ISAD)
00995           YYY = YMAX *RAN(ISAD)
00996           DO 493 ID = 1, NSEED
00997             DELS2 = (XS(ID)-XXX)**2 + (YS(ID)-YYY)**2
00998             IF (DELS2 .LT. RADI(ID)**2) GO TO 492
00999    493    CONTINUE
01000           NVOID = NVOID + 1
01001    492  CONTINUE
01002         EPSMC = (1. *NVOID) /NSHOT
01003   C
01004   C---  SUM POROSITY  ---
01005   C
01006         SUMV = 0.
01007         DIAMF = 0.
01008         DO 677 ID = 1, NSEED
01009           DIAM0(ID) = DIAM(ID)
01010           DIAMF = DIAMF + DIAM(ID)
01011           DELBX = MIN (XS(ID), XMAX-XS(ID))
01012           DELBY = MIN (YS(ID), YMAX-YS(ID))
01013           DELB = MIN (DELBX, DELBY)
01014           ABSD = MIN (ABS(DELB), RADI(ID))
01015           VID = PI *RADI(ID)**2
01016           IF (ABSD .LE. RADI(ID)) THEN
01017             THET = ACOS (ABSD /RADI(ID))
01018             VPIE = THET *RADI(ID)**2
01019             HGT = SQRT (RADI(ID)**2 - ABSD**2)
01020             VTRI = HGT *ABSD
01021             DELV = VPIE - VTRI
01022             IF (DELB .GT. 0.) THEN
01023               VID = VID - DELV
01024             ELSE
01025               VID = DELV
01026             ENDIF

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01027           ENDIF
01028           SUMV = SUMV + VID
01029    677  CONTINUE
01030         PORO = 1. - SUMV /XMAX /YMAX
01031         DIAMF = DIAMF /NSEED
01032         PRINT980,'PORO', PORO
01033   C
01034   C---  ROTATE SEEDS BY PI/2 IF REQUESTED
01035   C
01036         IF (IROTA .EQ. 1) THEN
01037           DO 1044 ID = 1, NSEED
01038             YTMP = XMAX - XS(ID)
01039             XS(ID) = YS(ID)
01040             YS(ID) = YTMP
```

```
01041    1044   CONTINUE
01042           XTMP = YMAX
01043           YMAX = XMAX
01044           XMAX = XTMP
01045         ENDIF
01046   C
01047   C---  INTERMEDIATE DUMP  ---
01048   C
01049         WRITE (99,*) NPAR,XMAX,YMAX,EPS0,DIAMF
01050         DO 692 ID = 1,NPAR
01051           WRITE(99,*) XS(ID),YS(ID),HITE(ID),DIAM(ID),RADI(ID)
01052    692  CONTINUE
01053   C
01054   C---  INITIALIZE PLOT  ---
01055   C
01056         XORIG = 0.
01057         YORIG = 0.
01058         RATXY = XMAX /YMAX
01059         IF (RATXY.GT.1.0) THEN
01060           XAXIS = 7.5
01061           YAXIS=XAXIS *0.95775 /RATXY
01062         ELSE
01063           XAXIS = 7.5 *RATXY
01064           YAXIS=XAXIS *0.95775 /RATXY
01065         ENDIF
01066         XSTP=(XMAX-XORIG)/1.
01067         YSTP=(YMAX-YORIG)/1.
01068   C
01069         CALL AREA2D(XAXIS,YAXIS)
01070         CALL GRAF(XORIG,XSTP,XMAX,YORIG,YSTP,YMAX)
01071         CALL FRAME
01072   C
01073         PRINT*,' '
01074         PRINT*,' '
01075         PRINT*,' '
01076         PRINT*,' '
01077         PRINT981,'NPAR',NPAR
01078         PRINT980,'XMAX',XMAX
01079         PRINT980,'YMAX',YMAX
01080         PRINT980,'EPS0',EPS0
01081         PRINT980,'PORO',PORO
01082         PRINT980,'EPSM',EPSMC
01083         PRINT980,'SPAC',SPAC

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01084         PRINT980,'DREF',DREF
01085   C
01086   C---  PLOTT SEEDS
01087   C
01088         IF (IPLTS.EQ.1) THEN
01089           CALL SCLPIC(0.5)
01090           CALL MARKER(18)
01091           CALL CURVE(XS,YS,NSEED,-1)
01092           CALL RESET('MARKER')
01093           CALL SCLPIC(1.)
01094         ENDIF
01095   C
01096         RJBAR=0.
01097         ABAR=0.
01098         NSUM=0
```

```
01099          NSUMOLD=0
01100          JLMAX=0
01101          JLMIN=200
01102          SUMLB=0.
01103          NBSUM=0
01104          DO 1621 K=1,20
01105    1621    FSID(K)=0
01106    C
01107          DO 1100 I=1,NSEED
01108    C
01109    C---   COMPUTE LINE CONSTANTS FOR Ith SEED  ---
01110    C
01111            JL=0
01112            DEMX=DEMAX0*1.6/SQRT(1.*NSEED)
01113            DO 1030 J=1,NSEED
01114              IF (I.EQ.J) GO TO 1030
01115              DELS = SQRT((XS(I)-XS(J))**2 + (YS(I)-YS(J))**2)
01116              IF (DELS.GT.DEMX) GO TO 1030
01117              JL = JL + 1
01118              X0(JL) = (XS(I)+XS(J)) /2.
01119              Y0(JL) = (YS(I)+YS(J)) /2.
01120              DELX = XS(J) - XS(I)
01121              DELY = YS(J) - YS(I)
01122              DELY = SIGN(MAX(ABS(DELY),1.E-8),DELY)
01123              SL(JL) = -DELX /DELY
01124              JB(JL) = J
01125    1030    CONTINUE
01126            NLIN = JL
01127    C
01128    C---   ADD BOUNDARY DOMAIN LINES  ---
01129    C
01130            EPS = 0.
01131            RRR = 0.5 + EPS
01132            DO 1040 J = 1, NBOX
01133    C
01134              THET = 2. *PI *(J-1)/NBOX - PI /2.
01135              X000 = (0.5 + RRR *COS(THET)) *XMAX
01136              Y000 = (0.5 + RRR *SIN(THET)) *YMAX
01137              SL00 = - 1. /SIGN (MAX (ABS(TAN(THET)),1.E-10), TAN(THET))
01138    C
01139    C---   REF: PURCEL PAGE 50
01140    C

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01141              BBB = 1.
01142              AAA = - SL00
01143              CCC = SL00 *X000 - Y000
01144              DELS = ABS(AAA*XS(I)+BBB*YS(I)+CCC)/SQRT(AAA**2+BBB**2)
01145              IF (DELS.GT.DEMX) GO TO 1040
01146              JL = JL + 1
01147              JB(JL) = - J
01148              X0(JL) = X000
01149              Y0(JL) = Y000
01150              SL(JL) = SL00
01151    1040    CONTINUE
01152            JLMAX = MAX (JL, JLMAX)
01153            JLMIN = MIN (JLMIN, JL)
01154    C
01155    C---   LOCATE NEAREST (PARTICLE) BOUNDING LINE  ---
01156    C
```

```
01157           DMIN = 1.E8
01158           EPS = 1.E-4 *SMEAS
01159           DO 1050 J = 1, NLIN
01160   C
01161   C---  NEW STUFF  ---
01162   C
01163             IF (X0(J).GT.XMAX-EPS .OR. X0(J).LT.EPS) GO TO 1050
01164             IF (Y0(J).GT.YMAX-EPS .OR. Y0(J).LT.EPS) GO TO 1050
01165             IF (JB(J) .GT. NSEED-NOUT) GO TO 1050
01166   C
01167             DELS=SQRT((XS(I)-X0(J))**2+(YS(I)-Y0(J))**2)
01168             IF (DELS.LT.DMIN) THEN
01169               DMIN=DELS
01170               JMN=J
01171             ENDIF
01172   1050      CONTINUE
01173   C
01174           JC=-1
01175           JN=JMN
01176           XX(1)=X0(JN)
01177           YY(1)=Y0(JN)
01178   C
01179   C---  START WALK AROUND CELL BOUNDARY  ---
01180   C
01181           KSAV=1
01182           NSYD=0
01183           MSID=0
01184           RAVE=0.
01185           RMIN=1.
01186           RMAX=0.
01187           ASUM=0.
01188           EPS = 1.E-2 *SMEAS
01189           DO 1110 K=1,20
01190   C
01191             JO=JC
01192             JC=JN
01193   C
01194             DMIN=SQRT(2.)
01195             XVJO=XX(K)
01196             YVJO=YY(K)
01197             DO 1120 J=1,JL

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01198   C
01199               IF (J.EQ.JC) GO TO 1120
01200               IF (J.EQ.JO) GO TO 1120
01201   C
01202               DSLO = SL(JC) - SL(J)
01203               DSLO = SIGN (MAX(ABS(DSLO),1.E-6), DSLO)
01204               XVJ=( (Y0(J)-SL(J)*X0(J))
01205        1              -(Y0(JC)-SL(JC)*X0(JC)) )/DSLO
01206               YVJ=Y0(JC)+SL(JC)*(XVJ-X0(JC))
01207               IF (ABS(SL(J)).LT.ABS(SL(JC))) THEN
01208                 YVJ=Y0(J)+SL(J)*(XVJ-X0(J))
01209               ENDIF
01210   C
01211   C---  NEW STUFF ---
01212   C
01213               IF (XVJ.GT.XMAX+EPS .OR. XVJ.LT.-EPS) GO TO 1120
01214               IF (YVJ.GT.YMAX+EPS .OR. YVJ.LT.-EPS) GO TO 1120
```

```
01215   C
01216   C---  CHECK FOR COUNTER-CLOCKWISE PATH  ---
01217   C     NOTE:  PUT THIS FIX IN BONZO
01218   C
01219               IF (JC .LE. NLIN) THEN
01220                 DIREC1 = (X0(JC)-XS(I)) *(YVJ-YVJO)
01221                 DIREC2 = (YS(I)-Y0(JC)) *(XVJ-XVJO)
01222               ELSE
01223                 DIREC1 = XVJ - XVJO
01224                 DIREC2 = YVJ - YVJO
01225                 IF (JB(JC).LT.-2) THEN
01226                   DIREC1 = - DIREC1
01227                   DIREC2 = - DIREC2
01228                 ENDIF
01229               ENDIF
01230               DIREC = DIREC1
01231               IF (ABS(DIREC2) .GT. ABS(DIREC1)) DIREC = DIREC2
01232               IF (DIREC. LT. 0.0) GO TO 1120
01233   C
01234               DVV=SQRT((XVJO-XVJ)**2+(YVJO-YVJ)**2)
01235               IF (DVV.LT.DMIN) THEN
01236                 JN=J
01237                 XX(K+1)=XVJ
01238                 YY(K+1)=YVJ
01239                 XSID(K,I)=XVJ
01240                 YSID(K,I)=YVJ
01241                 DMIN=DVV
01242                 DSXMIN=DSX
01243                 DVXMIN=DVX
01244                 DSVMIN=DSV
01245                 DSLOMIN=DSLO
01246               ENDIF
01247   1120      CONTINUE
01248             KSAV=KSAV+1
01249   C
01250   C---  COMPUTE BOND AND SIDE LENGTH  ---
01251   C
01252             IF (K.GT.1) THEN
01253               LSID(K-1,I)=SQRT((XX(K+1)-XX(K))**2+(YY(K+1)-YY(K))**2)
01254               NBSUM=NBSUM+1

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01255               IF (JC.GT.NLIN) THEN
01256                 LBON(K-1,I)=1.E10
01257                 NBSUM=NBSUM-1
01258               ELSE
01259                 L=JB(JC)
01260                 LBON(K-1,I)=SQRT((XS(I)-XS(L))**2+(YS(I)-YS(L))**2)
01261                 SUMLB=SUMLB+LBON(K-1,I)
01262               ENDIF
01263             ENDIF
01264   C
01265   C       COMPUTE AREA OF TRIANGULAR SEGMENT
01266   C
01267             IF (K.GT.1) THEN
01268               DELH=SQRT((XS(I)-X0(JC))**2+(YS(I)-Y0(JC))**2)
01269               DELB=SQRT((XX(K+1)-XX(K))**2+(YY(K+1)-YY(K))**2)
01270               IF (JC.GT.NLIN) THEN
01271                 BBB=1.
01272                 AAA=-SL(JC)
```

```
01273                 CCC=SL(JC)*X0(JC)-Y0(JC)
01274                 DELH=ABS(AAA*XS(I)+BBB*YS(I)+CCC)/SQRT(AAA**2+BBB**2)
01275               ENDIF
01276               ASUM=ASUM+0.5*DELH*DELB
01277             ENDIF
01278   C
01279             IF (K.GT.3 .AND. JC.EQ.JMN) GO TO 1130
01280   C
01281   C---  COMPUTE CORRESPONDENCE AND FLAG BOUNDARY SEEDS
01282   C
01283             IF (JN.GT.NLIN) THEN
01284               IPRM(K,I) = JB(JN)
01285               IF (IDBC(I).EQ.0) THEN
01286                 IDBC(I)=IPRM(K,I)
01287                 LBC(I)=K
01288               ELSEIF (IDBC(I).EQ.-1 .OR. IDBC(I).EQ.-3) THEN
01289                 IDBC(I)=IPRM(K,I)
01290                 LBC(I)=K
01291               ENDIF
01292   C
01293             ELSE
01294               IDP=JB(JN)
01295               IPRM(K,I)=IDP
01296               IF (IDP.LT.I) THEN
01297                 DO 1744 L=1,NSID(IDP)
01298                   IF (IPRM(L,IDP).EQ.I) THEN
01299                     LPRM(K,I)=L
01300                     LPRM(L,IDP)=K
01301                   ENDIF
01302   1744            CONTINUE
01303               ENDIF
01304             ENDIF
01305   C
01306             IF (JN.LE.NLIN) THEN
01307               XSJ=XS(JB(JN))
01308               YSJ=YS(JB(JN))
01309               DDSJ=SQRT((XS(I)-XSJ)**2+(YS(I)-YSJ)**2)
01310               RAVE=RAVE+DDSJ
01311               RMIN=MIN(RMIN,DDSJ)

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01312               RMAX=MAX(RMAX,DDSJ)
01313               CMIN=MIN(CMIN,DDSJ)
01314               CMAX=MAX(CMAX,DDSJ)
01315               MSID=MSID+1
01316             ENDIF
01317   C
01318             NSYD=NSYD+1
01319   C
01320   C---  PLOTT BONDS  ---
01321   C
01322             IF (IPLTB.EQ.1 .AND. JN.LE.NLIN) THEN
01323               XB(1)=XS(I)
01324               YB(1)=YS(I)
01325               XB(2)=XS(JB(JN))
01326               YB(2)=YS(JB(JN))
01327               CALL CURVE(XB,YB,2,1)
01328             ENDIF
01329   C
01330   1110    CONTINUE
```

```
01331   1130    CONTINUE
01332           RAVE=RAVE/MAX(MSID,1)
01333   C
01334   C---  COMPUTE SIDE AND AREA DIAGNOSTICS  ---
01335   C
01336           NSUM=NSUM+1
01337           RJBAR=RJBAR+NSYD
01338           FSID(NSYD)=FSID(NSYD)+1
01339           GAVE=GAVE+RAVE
01340           GMIN=GMIN+RMIN
01341           GMAX=GMAX+RMAX
01342           ABAR=ABAR+ASUM
01343   C
01344   C---  PLOTT CELL BOUNDARIES  ---
01345   C
01346           IF (IPLTC.EQ.1) THEN
01347             IF (YS(I) .LT. 0.5) THEN
01348             CALL CURVE(XX,YY,KSAV,0)
01349             CALL RESET ('DASH')
01350             ENDIF
01351           ENDIF
01352   C
01353           AREA(I)=ASUM
01354           NSID(I)=NSYD
01355   C
01356   1100  CONTINUE
01357   C
01358   C---  NUMBER NODES, ASSIGN X-Y COORDINATES, NODE CORRESPONDANCE AND
01359   C     FLAG BOUNDARY NODES  ---
01360   C
01361         IDN = 0
01362         DO 1400 ID=1,NSEED
01363           DO 1400 L=1,NSID(ID)
01364             IF (IDNOD(L,ID).EQ.0) THEN
01365   C
01366               IDN = IDN + 1
01367               XNOD(IDN) = XSID(L,ID)
01368               YNOD(IDN) = YSID(L,ID)

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01369               IDNOD(L,ID) = IDN
01370               IDP = IPRM(L,ID)
01371               IF (IDP.GT.0) THEN
01372                 LP = LPRM(L,ID)
01373                 LPP1 = MOD(LP,NSID(IDP))+1
01374                 IDNOD(LPP1,IDP) = IDN
01375               ENDIF
01376               LM1 = MOD(L+NSID(ID)-2,NSID(ID))+1
01377               IDP = IPRM(LM1,ID)
01378               IF (IDP.GT.0) THEN
01379                 LP = LPRM(LM1,ID)
01380                 IDNOD(LP,IDP) = IDN
01381               ENDIF
01382   C
01383               NODAR(8,IDN) = 0
01384               IDP = IPRM(L,ID)
01385               IDPM1 = IPRM(LM1,ID)
01386               IF (IDP.LT.0) NODAR(8,IDN) = IDP
01387               IF (IDPM1.LT.0) NODAR(8,IDN) = IDPM1
01388               IF (IDP.EQ.-IDBIN .OR. IDPM1.EQ.-IDBIN )
```

```
01389        1            NODAR(8,IDN) = -IDBIN
01390               IF (IDP.EQ.-IDBOU .OR. IDPM1.EQ.-IDBOU )
01391        1            NODAR(8,IDN) = -IDBOU
01392   C
01393             ENDIF
01394    1400 CONTINUE
01395         NNOD = IDN
01396   C
01397   C  NUMBER TUBES, IDENTIFY TUBE NODES, LENGTHS AND DIAMETERS
01398   C  ASSIGN TUBE ENDPOINTS AND XY SHIFTS
01399   C
01400    1610 IDT = 0
01401         DO 1402 ID=1,NSEED
01402           DO 1402 L=1,NSID(ID)
01403             IDP = IPRM(L,ID)
01404             IF (IDP.GT.ID .OR. IDP.LT.0) THEN
01405   C
01406               IDT = IDT + 1
01407               TUBNOD(1,IDT) = IDNOD(L,ID)
01408               TUBNOD(3,IDT) = ID
01409               TUBNOD(4,IDT) = IDP
01410               LP1 = MOD(L,NSID(ID))+1
01411               TUBNOD(2,IDT) = IDNOD(LP1,ID)
01412               TUBAR(1,IDT) = MAX (LSID(L,ID),1.E-6*XMAX)
01413               TUBAR(9,IDT) = 1.* IDP
01414               IDTUB(L,ID) = IDT
01415               IF (IDP.GT.0) THEN
01416                 LP = LPRM(L,ID)
01417                 IDTUB(LP,IDP) = IDT
01418                 DEL=SQRT( (XS(ID)-XS(IDP))**2 + (YS(ID)-YS(IDP))**2 )
01419                 IF (IREDU.EQ.1) THEN
01420                   TUBAR(2,IDT) = DEL - RADI(ID) - RADI(IDP) - DELDIA
01421                 ELSEIF (IREDU.EQ.2) THEN
01422                   TUBDI = DEL - RADI(ID) - RADI(IDP)
01423                   TUBAR(2,IDT) = TUBDI *(1. - DELDIA)
01424                 ELSEIF (IREDU.EQ.3) THEN
01425                   TUBDI = DEL - RADI(ID) - RADI(IDP)

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01426                   TUBAR(2,IDT) = TUBDI /(1. + DELDIA*TUBDI)
01427                 ENDIF
01428               ELSE
01429                 IF (IDP .EQ. -1) DEL = YS(ID)
01430                 IF (IDP .EQ. -2) DEL = XMAX - XS(ID)
01431                 IF (IDP .EQ. -3) DEL = YMAX - YS(ID)
01432                 IF (IDP .EQ. -4) DEL = XS(ID)
01433                 IF (IREDU.EQ.1) THEN
01434                   TUBAR(2,IDT) = DEL - RADI(ID) - DELDIA/2.
01435                 ELSEIF (IREDU.EQ.2) THEN
01436                   TUBDI = DEL - RADI(ID)
01437                   TUBAR(2,IDT) = TUBDI *(1. - DELDIA)
01438                 ELSEIF (IREDU.EQ.3) THEN
01439                   TUBDI = DEL - RADI(ID)
01440                   TUBAR(2,IDT) = TUBDI /(1. + TUBDI*DELDIA)
01441                 ENDIF
01442               ENDIF
01443               KBLOC(IDT) = 1
01444               IF (TUBAR(2,IDT) .LT. 1.E-8*XMAX) THEN
01445                 KBLOC(IDT) = 0
01446                 TUBAR(2,IDT) = 1.E-8 *XMAX
```

```
01447                ENDIF
01448   C
01449                IF (IDP.GT.0) THEN
01450                  DEL=SQRT( (XS(ID)-XS(IDP))**2 + (YS(ID)-YS(IDP))**2 )
01451                  DELTA = (RADI(ID)-RADI(IDP))/2.
01452                  DXDL=(XS(IDP)-XS(ID))/DEL
01453                  DYDL=(YS(IDP)-YS(ID))/DEL
01454                  DELTAX = DELTA *DXDL
01455                  DELTAY = DELTA *DYDL
01456                ELSE
01457                  DELTAX = 0.
01458                  DELTAY = 0.
01459                  IF (IDP .EQ. -1) DELTAY = TUBAR(2,IDT) /2.
01460                  IF (IDP .EQ. -2) DELTAX = - TUBAR(2,IDT) /2.
01461                  IF (IDP .EQ. -3) DELTAY = - TUBAR(2,IDT) /2.
01462                  IF (IDP .EQ. -4) DELTAX = TUBAR(2,IDT) /2.
01463                ENDIF
01464                TUBAR(3,IDT) = XSID(L,ID) + DELTAX
01465                TUBAR(4,IDT) = YSID(L,ID) + DELTAY
01466                TUBAR(5,IDT) = XSID(L+1,ID) + DELTAX
01467                TUBAR(6,IDT) = YSID(L+1,ID) + DELTAY
01468                TUBAR(7,IDT) = DELTAX
01469                TUBAR(8,IDT) = DELTAY
01470   C
01471              ENDIF
01472   1402   CONTINUE
01473          NTUB = IDT
01474   C
01475   C---   IDENTIFY NODE TRIOS AND ASSOCIATED TUBE NUMBERS  ---
01476   C      SEQUENCE OF TRIOS IS IN ANTI-CLOCKWISE DIRECTION
01477   C
01478          DO 1406 ID=1,NSEED
01479            DO 1406 L=1,NSID(ID)
01480              IDP = IPRM(L,ID)
01481              IF (IDP.GT.ID .OR. IDP.LT.0) THEN
01482                IDN = IDNOD(L,ID)

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01483                IF (NODAR(1,IDN).EQ.0) THEN
01484                  LP1 = MOD(L,NSID(ID))+1
01485                  LM1 = MOD(L+NSID(ID)-2,NSID(ID))+1
01486                  NODAR(2,IDN) = IDNOD(LP1,ID)
01487                  NODAR(3,IDN) = IDNOD(LM1,ID)
01488                  NODAR(5,IDN) = IDTUB(L,ID)
01489                  NODAR(6,IDN) = IDTUB(LM1,ID)
01490                  NODAR(9,IDN) = ID
01491                  NODAR(10,IDN) = IPRM(L,ID)
01492                  NODAR(11,IDN) = IPRM(LM1,ID)
01493                  NODAR(1,IDN) = 2
01494                  IDP = IPRM(L,ID)
01495                  IF (IDP.GT.0) THEN
01496                    LP = LPRM(L,ID)
01497                    LPP1 = MOD(LP,NSID(IDP))+1
01498                    IF (IDNOD(L,ID).EQ.IDNOD(LPP1,IDP)) THEN
01499                      LPP2 = MOD(LPP1,NSID(IDP))+1
01500                      NODAR(4,IDN) = IDNOD(LPP2,IDP)
01501                      NODAR(7,IDN) = IDTUB(LPP1,IDP)
01502                      NODAR(1,IDN) = 3
01503                      GO TO 1406
01504                    ENDIF
```

```
01505                 ENDIF
01506                 IDP = IPRM(LM1,ID)
01507                 NODAR(10,IDN) = IDP
01508                 IF (IDP.GT.0) THEN
01509                   LP = LPRM(LM1,ID)
01510                   IF (IDNOD(L,ID).EQ.IDNOD(LP,IDP)) THEN
01511                     LPM1 = MOD(LP+NSID(IDP)-2,NSID(IDP))+1
01512                     NODAR(4,IDN) = IDNOD(LPM1,IDP)
01513                     NODAR(7,IDN) = IDTUB(LPM1,IDP)
01514                     NODAR(1,IDN) = 3
01515                   ENDIF
01516                 ENDIF
01517               ENDIF
01518             ENDIF
01519    1406 CONTINUE
01520   C
01521   C---  TABULATE AND STORE BOUNDARY NODES AND CROSSING TUBES  ---
01522   C     NNBC(J) IS THE NUMBER OF NODES/TUBES ON BOUNDARY J; NBID(I,J) IS
01523   C     THE NODE NODE NUMBER OF THE JTH NODE ON BOUNDARY I; TBID(I,J) IS
01524   C     THE TUBE NUMBER OF THE JTH TUBE CROSSING BOUNDARY I.
01525   C
01526         NNBC(1) = 0
01527         NNBC(2) = 0
01528         NNBC(3) = 0
01529         NNBC(4) = 0
01530         DO 1447 IDN = 1, NNOD
01531           IDB = - NODAR(8,IDN)
01532           IF (IDB .GT. 0) THEN
01533             NNBC(IDB) = NNBC(IDB) + 1
01534             NBID(IDB,NNBC(IDB)) = IDN
01535             DO 1448 J = 1, NODAR(1,IDN)
01536               IDNJ = NODAR(1+J,IDN)
01537               IF (NODAR(8,IDN) .NE. NODAR(8,IDNJ)) THEN
01538                 TBID(IDB,NNBC(IDB)) = NODAR(4+J,IDN)
01539                 GO TO 1447

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01540               ENDIF
01541    1448     CONTINUE
01542           ENDIF
01543    1447 CONTINUE
01544   C
01545   C---  PLOTT PARTICLES
01546   C
01547         IF (IPLTP.EQ.1) THEN
01548           DO 1811 ID = 1, NSEED
01549             XCEN = XS(ID) *XAXIS /XMAX
01550             YCEN = YS(ID) *YAXIS /YMAX
01551             RADIN = 0.95 *RADI(ID) *XAXIS /XMAX
01552             CALL BLCIR (XCEN, YCEN, RADIN, 0)
01553    1811   CONTINUE
01554         ENDIF
01555   C
01556         IF (IPLTP.NE.0) THEN
01557           IF (IPLTP .EQ. 1) THEN
01558             CALL MARKER(16)
01559   CXXX         CALL BLSYM
01560           ELSEIF (IPLTP .EQ. -1) THEN
01561             CALL MARKER(15)
01562           ENDIF
```

```
01563           CALL BLREC(-0.2*XAXIS,-0.2*YAXIS,0.2*XAXIS,1.4*YAXIS,0)
01564           CALL BLREC(-0.2*XAXIS,-0.2*YAXIS,1.4*XAXIS,0.2*YAXIS,0)
01565           CALL BLREC( 1.0*XAXIS,-0.2*YAXIS,0.2*XAXIS,1.4*YAXIS,0)
01566           CALL BLREC(-0.2*XAXIS, 1.0*YAXIS,1.4*XAXIS,0.2*YAXIS,0)
01567           DO 1801 ID=1,NSEED
01568             XB(1)=XS(ID)
01569             YB(1)=YS(ID)
01570             FAC= 2.* RADI(ID)/XMAX *XAXIS/0.082
01571             CALL SCLPIC(FAC)
01572             CALL CURVE(XB,YB,1,1)
01573    1801   CONTINUE
01574           CALL SCLPIC(1.)
01575           CALL RESET('BLSYM')
01576         ENDIF
01577   C
01578   C---  COMPUTE MAX NODE DIAMETERS  ---
01579   C
01580           DO 3018 IDN = 1, NNOD
01581             XTU(IDN) = XNOD(IDN)
01582             YTU(IDN) = YNOD(IDN)
01583             RTU(IDN) = XMAX /100.
01584             RMIN = XMAX
01585   C         IF (NODAR(1,IDN) .LT. 3) GO TO 3018
01586             DO 3019 J = 1, NODAR(1,IDN)
01587               IDT = NODAR (4+J, IDN)
01588               ID = TUBNOD (3, IDT)
01589               IDP = TUBNOD (4, IDT)
01590               IF (ID.GT.0 .AND. IDP.GT.0 ) THEN
01591                 XAA(J,1) = -2. *(XS(ID) - XS(IDP))
01592                 XAA(J,2) = -2. *(YS(ID) - YS(IDP))
01593                 XAA(J,3) = -2. *(RADI(ID) - RADI(IDP))
01594                 RHS(J) = RADI(ID)**2 - RADI(IDP)**2
01595        1           - XS(ID)**2 + XS(IDP)**2 - YS(ID)**2 + YS(IDP)**2
01596                 QHS(J) = RADI(ID) - RADI(IDP)

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01597                 DIS = SQRT ((XS(ID)-XS(IDP))**2 + (YS(ID)-YS(IDP))**2)
01598                 RTRY = DIS - RADI(ID) - RADI(IDP)
01599                 RMIN = MIN (RMIN, RTRY)
01600               ELSE
01601                 XAA(J,1) = 0.
01602                 XAA(J,2) = 0.
01603                 XAA(J,3) = 0.
01604                 RHS(J) = 0.
01605                 QHS(J) = 0.
01606                 IDSAV = ID
01607                 ID = MAX (ID, IDP)
01608                 IDP = MIN (IDSAV, IDP)
01609                 IF (IDP .EQ. -2 .OR. IDP .EQ. -4) THEN
01610                   XAA(J,1) = 1.
01611                   RHS(J) = 0.
01612                   IF (IDP .EQ. -2) RHS(J) = XMAX
01613                 ELSE
01614                   XAA(J,2) = 1.
01615                   RHS(J) = 0.
01616                   IF (IDP .EQ. -3) RHS(J) = YMAX
01617                 ENDIF
01618               ENDIF
01619    3019     CONTINUE
01620   C
```

```
01621              WT = 1.
01622              WTR = 0.3
01623              RTU(IDN) = 1.1 *RMIN
01624              RNEW = RTU(IDN)
01625              ITSK = 0
01626              DO 3077 ITS = 1, 50
01627                ITSK = ITSK + 1
01628    C
01629                RTU(IDN) = (1.-WTR) *RTU(IDN) + WTR *RNEW
01630                DETA = XAA(1,1) *XAA(2,2) - XAA(1,2) *XAA(2,1)
01631                XHS(1) = RHS(1) + 2.* QHS(1) *RTU(IDN)
01632                XHS(2) = RHS(2) + 2.* QHS(2) *RTU(IDN)
01633                DETX = XHS(1)   *XAA(2,2) - XAA(1,2) *XHS(2)
01634                DETY = XAA(1,1) *XHS(2)  - XHS(1)   *XAA(2,1)
01635                XNEW = DETX /DETA
01636                YNEW = DETY /DETA
01637                XTU(IDN) = (1.-WT) *XTU(IDN) + WT *XNEW
01638                YTU(IDN) = (1.-WT) *YTU(IDN) + WT *YNEW
01639    C
01640                DELM = 0.
01641                ERR = 0.
01642                DO 3076 J = 1, NODAR(1,IDN)
01643                  ID = NODAR(J+8,IDN)
01644                  IF (ID .LT. 1) GO TO 3076
01645                  RTUF = (XS(ID)-XTU(IDN))**2 + (YS(ID)-YTU(IDN))**2
01646                  RXX = SQRT (RTUF) - RADI(ID)
01647                  RES(J) = SQRT(RTUF) - RADI(ID) - RTU(IDN)
01648                  ERR = MAX (ERR, ABS(RES(J)))
01649                  IF (ABS(RXX-RTU(IDN)) .GT. DELM) THEN
01650                    DELM = ABS (RXX-RTU(IDN))
01651                    RNEW = RXX
01652                  ENDIF
01653     3076       CONTINUE

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01654                IF (ERR .LT. 1.E-6*XMAX) GO TO 3078
01655    C
01656     3077      CONTINUE
01657     3078      CONTINUE
01658              RTU(IDN) = MAX (RTU(IDN), 1.E-30)
01659    C
01660     3018    CONTINUE
01661    C
01662    C---  COMPUTE EFFECTIVE PORE RADII  ---
01663    C
01664            PORSUM = 0.
01665            DO 3017 IDN = 1, NNOD
01666              APORE(IDN) = 0.
01667              DO 3016 J = 1, NODAR(1,IDN)
01668                IDT = NODAR (4+J, IDN)
01669                ID = TUBNOD (3, IDT)
01670                IDP = TUBNOD (4, IDT)
01671                IF (ID.GT.0 .AND. IDP.GT.0 ) THEN
01672                  BASE2 = (XS(ID)-XS(IDP))**2 + (YS(ID)-YS(IDP))**2
01673                  BASE = SQRT (BASE2)
01674                  RLEG = BASE /2.
01675                  XMID = (XS(ID) + XS(IDP)) /2.
01676                  YMID = (YS(ID) + YS(IDP)) /2.
01677                  HIGHT2 = (XNOD(IDN)-XMID)**2 + (YNOD(IDN)-YMID)**2
01678                  HIGHT = SQRT (HIGHT2)
```

```
01679                 DTHETA = ATAN (HIGHT /RLEG)
01680                 IF (RADI(ID)+RADI(IDP) .LE. BASE) THEN
01681                   APART = DTHETA /2. *(RADI(ID)**2 + RADI(IDP)**2)
01682                 ELSE
01683                   RLAP = (RADI(ID) + RADI(IDP) - BASE) /2.
01684                   PHI1 = ACOS ((RADI(ID)-RLAP) /RADI(ID))
01685                   HLAP = RADI(ID) *SIN (PHI1)
01686                   PHI2 = ACOS ((RADI(IDP)-RLAP) /RADI(IDP))
01687                   ATRI = (RADI(ID)-RLAP) *HLAP /2.
01688                   APART = (DTHETA-PHI1) /2. *RADI(ID)**2 + ATRI
01689                   ATRI = (RADI(IDP)-RLAP) *HLAP /2.
01690                   APART = APART + (DTHETA-PHI2)/2. *RADI(IDP)**2 + ATRI
01691                 ENDIF
01692                 DAREA = MAX (0., HIGHT *RLEG - APART)
01693               ELSE
01694                 IDSAV = ID
01695                 ID = MAX (ID, IDP)
01696                 IDP = MIN (IDSAV, IDP)
01697                 HYPOT2 = (XS(ID)-XNOD(IDN))**2 + (YS(ID)-YNOD(IDN))**2
01698                 HYPOT = MAX (1.E-10*XMAX, SQRT (HYPOT2))
01699                 IF (IDP/2*2 .EQ. IDP) THEN
01700                   RLEG = ABS (YS(ID) - YNOD(IDN))
01701                 ELSE
01702                   RLEG = ABS (XS(ID) - XNOD(IDN))
01703                 ENDIF
01704                 HIGHT = SQRT (HYPOT2 - RLEG**2)
01705                 DTHETA = PI /2. - ACOS (RLEG /HYPOT)
01706                 IF (RADI(ID) .LE. HIGHT) THEN
01707                   APART = DTHETA /2. *RADI(ID)**2
01708                 ELSE
01709                   RLAP = RADI(ID) - HIGHT
01710                   PHI = ACOS ((RADI(ID)-RLAP) /RADI(ID))

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01711                   HLAP = RADI(ID) *SIN (PHI)
01712                   ATRI = (RADI(ID)-RLAP) *HLAP /2.
01713                   APART = (DTHETA-PHI) /2. *RADI(ID)**2 + ATRI
01714                 ENDIF
01715                 DAREA = MAX (0., HIGHT *RLEG /2. - APART)
01716               ENDIF
01717               APORE(IDN) = APORE(IDN) + DAREA
01718    3016      CONTINUE
01719             PORSUM = PORSUM + APORE(IDN)
01720    3017    CONTINUE
01721           EPSVOID = PORSUM /(XMAX*YMAX)
01722   C
01723   C---  PLOTT NODES  ---
01724   C
01725         IF (IPLTN.NE.0) THEN
01726           DO 1809 IDN = 1,NNOD
01727             XSHIF = 0.
01728             YSHIF = 0.
01729             FAC = 1.
01730             IF (NODAR(8,IDN).EQ.0) THEN
01731               SIZ = 0.
01732               DSHIF = 0.
01733               DO 1808 J=1,NODAR(1,IDN)
01734                 IDT = NODAR(4+J,IDN)
01735                 XSHIF = XSHIF + TUBAR(7,IDT)
01736                 YSHIF = YSHIF + TUBAR(8,IDT)
```

```
01737                 DSHIF = DSHIF + SQRT(TUBAR(7,IDT)**2 + TUBAR(8,IDT)**2)
01738                 SIZ = SIZ + TUBAR(2,IDT)
01739    1808       CONTINUE
01740               XSHIF = XSHIF /NODAR(1,IDN)
01741               YSHIF = YSHIF /NODAR(1,IDN)
01742               SIZ = SIZ /NODAR(1,IDN)
01743               FAC = 0.8 *MIN(DSHIF,SIZ) /XMAX *XAXIS /0.082
01744             ENDIF
01745             FAC = MAX (FAC, .01)
01746             XB(1) = XNOD(IDN) + XSHIF
01747             YB(1) = YNOD(IDN) + YSHIF
01748             IF (IPLTN.NE.1) FAC = 1.
01749   C
01750             CALL SCLPIC(FAC)
01751   C
01752             XB(1) = XTU(IDN)
01753             YB(1) = YTU(IDN)
01754             FAC = 2. *RTU(IDN) /XMAX *XAXIS /0.082
01755             FAC = MAX (FAC, 0.01)
01756             FAC = MIN (FAC, 0.2 *XMAX /XMAX *XAXIS /0.082 )
01757             CALL SCLPIC(FAC)
01758             CALL MARKER(15)
01759
01760   C         CALL SCLPIC(0.5)
01761             CALL CURVE(XB,YB,1,1)
01762    1809   CONTINUE
01763           CALL SCLPIC(1.)
01764         ENDIF
01765   C
01766   C   PLOTT TUBES
01767   C

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01768         IF (IPLTT.NE.0) THEN
01769         CALL BLREC(-0.2*XAXIS,-0.2*YAXIS,0.2*XAXIS,1.4*YAXIS,0)
01770         CALL BLREC(-0.2*XAXIS,-0.2*YAXIS,1.4*XAXIS,0.2*YAXIS,0)
01771         CALL BLREC( 1.0*XAXIS,-0.2*YAXIS,0.2*XAXIS,1.4*YAXIS,0)
01772         CALL BLREC(-0.2*XAXIS, 1.0*YAXIS,1.4*XAXIS,0.2*YAXIS,0)
01773         DO 1803 IDT=1,NTUB
01774           XB(1) = TUBAR(3,IDT)
01775           YB(1) = TUBAR(4,IDT)
01776           XB(2) = TUBAR(5,IDT)
01777           YB(2) = TUBAR(6,IDT)
01778           WID = MIN (TUBAR(2,IDT), 3.*TUBAR(1,IDT))
01779           IF (TUBAR(2,IDT) .LT. 1.1E-2 *SPAC) WID = 0.
01780           WID = 0.98 *MAX (WID, 0.)
01781           WID = WID /XMAX *XAXIS
01782           IF (IPLTT.EQ.1) CALL THKCRV(WID)
01783           CALL CURVE(XB,YB,2,0)
01784    1803 CONTINUE
01785         CALL RESET('THKCRV')
01786         ENDIF
01787   C
01788   C---  PLOTT TUBE/NODE  TRIOS  ---
01789   C
01790         IPLTTRI = 0
01791         IF (IPLTTRI.NE.0) THEN
01792         DO 1793 IDN = 1, NNOD
01793           XB(1) = XNOD(IDN)
01794           YB(1) = YNOD(IDN)
```

```
01795           ICH = NODAR(1,IDN)
01796           DO 1793 J = 1, ICH
01797             ID = NODAR(J+1,IDN)
01798             XB(2) = XNOD(ID)
01799             YB(2) = YNOD(ID)
01800             CALL CURVE(XB,YB,2,0)
01801    1793 CONTINUE
01802         CALL RESET('DASH')
01803         ENDIF
01804   C
01805   C   SHADE BACKGROUND
01806   C
01807         IF (ISHAD.NE.0) THEN
01808           IF (XBA1(2).LT.0.9) THEN
01809             XBA1(1) = 0.
01810             YBA1(1) = 0.
01811             XBA1(2) = XMAX
01812             YBA1(2) = 0.
01813             XBA2(1) = 0.
01814             YBA2(1) = YMAX
01815             XBA2(2) = XMAX
01816             YBA2(2) = YMAX
01817           ENDIF
01818           CALL SHDPAT (17)
01819           IF (ISHAD .LT. 0) CALL SHDPAT(16)
01820           CALL SHDCRV(XBA1,YBA1,2,XBA2,YBA2,2)
01821         ENDIF
01822   C
01823         CALL ENDPL(0)
01824         PRINT*,ISEED0

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01825         PRINT913,NPAR
01826         PRINT913,NNOD
01827         PRINT913,NTUB
01828         PRINT900,PORO
01829         PRINT980,'EPSV',EPSVOID
01830         PRINT*,' '
01831   C
01832   C   CHECK CONSISTANCY
01833   C
01834         IPAS = 1
01835         DO 502 IDN = 1,NNOD
01836           DO 503 L = 1,NODAR(1,IDN)
01837             NUM = NODAR(L+1,IDN)
01838             IDT = NODAR(L+4,IDN)
01839             L2OK = 0
01840             NOK = 0
01841             DO 504 L2 = 1,NODAR(1,NUM)
01842               IF (NODAR(L2+1,NUM) .EQ. IDN) THEN
01843                 L2OK = L2
01844                 NOK = NOK + 1
01845               ENDIF
01846    504        CONTINUE
01847             IF (NOK .EQ. 0) THEN
01848               IPAS = 0
01849               PRINT*,'NO NODE CORRESPONDANCE'
01850               PRINT1904,IDN,NUM,L,IDT,XNOD(IDN),YNOD(IDN)
01851               DO 465 IKL = 1, NODAR(1,NUM)
01852                 N2 = NODAR(IKL+1,NUM)
```

```
01853    465          PRINT1903,IKL,N2,NODAR(IKL+4,N2),XNOD(N2),YNOD(N2)
01854              ELSEIF (NOK .EQ. 1) THEN
01855                IDT2 = NODAR(L2OK+4,NUM)
01856                IF (IDT .NE. IDT2) THEN
01857                  IPAS = 0
01858                  PRINT*,'NO TUBE CORRESPONDANCE'
01859                  PRINT1910,IDN,NODAR(1,IDN),L,IDT,
01860         1                  NUM,NODAR(1,NUM),L2OK,IDT2
01861                ENDIF
01862              ELSE
01863                IPAS = 0
01864                PRINT*,'MULTIPLE NODE CORRESPONDANCE'
01865              ENDIF
01866    503     CONTINUE
01867    502   CONTINUE
01868          IF (IPAS .EQ. 1) PRINT*,' CORRESPONDANCE IS OK'
01869          PRINT*,'INPUT ICONT   1 = CONT  2 = RESTART'
01870          READ*,ICONT
01871          IF (ICONT.EQ.2) GO TO 1600
01872    C
01873    C---  COMPUTE TUBE DIAGNOSTICS  ---
01874    C
01875          SUMT = 0.
01876          NSUM = 0
01877          DMAX = 0.
01878          DO 1771 IDT = 1, NTUB
01879            IDBOUN = MIN (TUBNOD(3,IDT), TUBNOD(4,IDT))
01880            IF (IDBOUN .GT. 0) THEN
01881              NSUM = NSUM + 1

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01882                SUMT = SUMT + TUBAR(2,IDT)
01883                DMAX = MAX (DMAX, TUBAR(2,IDT))
01884              ENDIF
01885     1771 CONTINUE
01886          DTBAR = SUMT /NSUM
01887    C
01888          SDEVT = 0.
01889          IFRE = NTUB /20
01890          DO 1773 IBIN = 1,IFRE
01891     1773   FREQ(IBIN) = 0.
01892    C
01893          DTMIN = 0.
01894          DTMAX = 2.*DTBAR
01895          DO 1772 IDT = 1,NTUB
01896            IDBOUN = MIN (TUBNOD(3,IDT), TUBNOD(4,IDT))
01897            IF (IDBOUN .GT. 0) THEN
01898              SDEVT = SDEVT + (TUBAR(2,IDT)-DTBAR)**2
01899              IBIN = NINT((IFRE-1.)*(TUBAR(2,IDT)-DTMIN)/(DTMAX-DTMIN)) + 1
01900              FREQ(IBIN) = FREQ(IBIN) + 1.
01901            ENDIF
01902     1772 CONTINUE
01903          SDEVT = SQRT(SDEVT /NSUM)
01904          PRINT981,'NSUM',NSUM
01905          PRINT981,'NBOU',NTUB-NSUM
01906          PRINT980,'DBAR',DTBAR
01907          PRINT980,'SDEV',SDEVT
01908    C
01909          PRINT900,DMAX
01910          WRITE(15,901) IFRE
```

```
01911         DO 1774 IBIN = 1, IFRE
01912           FSUM = 0.
01913           DO 1788 II = 1, IBIN
01914    1788     FSUM = FSUM + FREQ(II)
01915           FSUM = FSUM /NSUM
01916           FDIS = 1. *FREQ(IBIN) /NSUM /(1./IFRE)
01917           WRITE(15,900) (IBIN-0.5)/IFRE, FDIS, FSUM
01918    1774   PRINT901,IBIN, FDIS, FSUM
01919    C
01920    C---   COMPUTE BOUNDARY LENGTHS  ---
01921    C
01922         DO 1776 J=1,NBOX
01923    1776    LBOUN(J)=0.
01924         DO 1777 I=1,NSEED
01925           IBOU=-IDBC(I)
01926           IF (IBOU.GT.0) THEN
01927             LB=LBC(I)
01928             LBOUN(IBOU)=LBOUN(IBOU)+LSID(LB,I)
01929           ENDIF
01930    1777   CONTINUE
01931    C
01932    C---   COMPUTE PERIMETER AND PROJECTED AREAS  ---
01933    C
01934         DO 1778 I=1,NSEED
01935           PERI(I)=0.
01936           APRX(I)=0.
01937           APRY(I)=0.
01938           DO 1778 L=1,NSID(I)

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01939             PERI(I)=PERI(I)+LSID(L,I)
01940             IDP=IPRM(L,I)
01941             IF (IDP.LT.0) THEN
01942               THET=-PI/2.+(-IDP-1)*2.*PI/NBOX
01943               DXDL=COS(THET)
01944               DYDL=SIN(THET)
01945             ELSE
01946               DXXX=XS(IDP)-XS(I)
01947               DYYY=YS(IDP)-YS(I)
01948               DLLL=SQRT(DXXX**2+DYYY**2)
01949               DXDL=DXXX/DLLL
01950               DYDL=DYYY/DLLL
01951             ENDIF
01952             APRX(I)=APRX(I)+LSID(L,I)*ABS(DXDL)/2.
01953             APRY(I)=APRY(I)+LSID(L,I)*ABS(DYDL)/2.
01954    1778   CONTINUE
01955    C
01956         DO 1785 I=1,NSEED
01957    1785       IF (IDBC(I).LT.-NBOX) PRINT902,I,IDBC(I),XS(I),YS(I)
01958    C
01959         CKSUM=0.
01960         PRINT*,NSEED
01961         DO 1631 K=1,20
01962           CKSUM=CKSUM+(1.*K)*(1.*FSID(K))/NSUM
01963    1631   PRINT902,K,FSID(K),(1.*FSID(K))/NSUM
01964         PRINT902,JLMIN,JLMAX
01965         GAVE=GAVE/NSUM*SQRT(1.*NSEED)
01966         GMIN=GMIN/NSUM*SQRT(1.*NSEED)
01967         GMAX=GMAX/NSUM*SQRT(1.*NSEED)
01968         CMIN=CMIN*SQRT(1.*NSEED)
```

```
01969         CMAX=CMAX*SQRT(1.*NSEED)
01970   C
01971         PRINT900,CMIN
01972         PRINT900,GMIN
01973         PRINT900,GAVE
01974         PRINT900,GMAX
01975         PRINT900,CMAX
01976         READ*
01977   2000  CONTINUE
01978   C
01979   C---  PRINT NODE/TUBE CORRESPONDANCE STUFF  ---
01980   C
01981         DO 1733 IDN = 1, 0 *NNOD
01982           ICH = NODAR(1,IDN)
01983           DO 1733 J = 1, ICH
01984             IDT = NODAR(4+J,IDN)
01985             PRINT904,IDN,NODAR(1+J,IDN),TUBNOD(1,IDT),TUBNOD(2,IDT)
01986    1733 CONTINUE
01987   C
01988   C---  BEGIN CALCULATIONS OF PRESSURE FIELD  ---
01989   C
01990   1620  PIN = 1000.
01991         PEX = 1.
01992         TMP = 298.
01993         RGAS = 287.
01994         PRINT*,'INPUT PIN,PEX',PIN,PEX
01995         READ*,PIN,PEX

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01996         NSOR = 1000
01997         WGT = 0.5
01998         PRINT*,'INPUT NSOR, WGT',NSOR,WGT
01999         READ*,NSOR,WGT
02000         ABSERR = 1.E-20
02001         RELERR = 1.E-8
02002         PRINT*,'INPUT ABSERR,RELERR',ABSERR,RELERR
02003         READ*,ABSERR,RELERR
02004         IPLTPR = 0
02005         IPLTPF = 0
02006         IPLTPFY = 0
02007         IF (IDBIN .NE. IDBEV) THEN
02008           IPLTPF = 0
02009           IPLTPFY = 0
02010         ENDIF
02011         PRINT*,'INPUT IPLTPR,IPLTPF,IPLTFY',IPLTPR,IPLTPF,IPLTPFY
02012         READ*,IPLTPR,IPLTPF,IPLTPFY
02013         ICOMP = 0
02014         PRINT*,'INPUT ICOMP:  0 = INCOMP  1 = COMP',ICOMP
02015         READ*,ICOMP
02016         KPAR = 300
02017         DTSTR = 0.5
02018         PRINT*,'INPUT NUMBER OF TRACER PARTICLES AND TIME',KPAR,DTSTR
02019         READ*,KPAR,DTSTR
02020         PECL = 1.E10
02021         ISED = 12344321
02022         IF (KPAR .GT. 0) THEN
02023           PRINT*,'INPUT PECLET NUMBER',PECL
02024           READ*,PECL
02025           IMICF = 0
02026           PRINT*,'SPATIAL DIST OR MICRO-FINGERS ?  0 = DIST  1 = MF',IMICF
```

```
02027           READ*,IMICF
02028           IPARA = 1
02029           PRINT*,'PARABOLIC VEL PROFILE ?  0 = NO  1 = YES',IPARA
02030           READ*,IPARA
02031           IMIX = 0
02032           PRINT*,'MIX NODE STREAMLINES ?  0 = NO  1 = YES', IMIX
02033           READ*,IMIX
02034           IUNI = 0
02035           PRINT*,'UNIFORM PARTICLE DIST IN INLET TUBE ?  0 = NO  1 = YES',
02036        1            IUNI
02037           READ*,IUNI
02038           IRANS = 0
02039           PRINT*,'RANDOMIZE STREAMLINE AT EVERY STEP ?,  0 = NO  1 = YES',
02040        1            IRANS
02041           READ*,IRANS
02042           IZZZ = 0
02043           PRINT*,'EXIT TUBE ON ENTRANCE STREAMLINE ?  0 = NO  1 = YES',
02044        1            IZZZ
02045           READ*,IZZZ
02046           IPLTTR = 0
02047           IF (IMICF .NE. 1) THEN
02048             PRINT*,'PARTICLE TRACES ?  0 = NO  1 = YES',IPLTTR
02049             READ*,IPLTTR
02050           ENDIF
02051           PRINT*,'INPUT SEED FOR TRACER INJECTION',ISED
02052           READ*,ISED

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02053         ENDIF
02054         IPRINI = 1
02055         IF (IMETH .LT. 0) IPRINI = 0
02056         IF (ICONT .NE. 0) IPRINI = 0
02057         PRINT*,'DO YOU WANT PRESSURES (RE)INITIALIZED',IPRINI
02058         READ*,IPRINI
02059         XXX0 = 0.5
02060         EDGE = 0.
02061         PRINT*,'INPUT XXX0, EDGE',XXX0,EDGE
02062         READ*,XXX0,EDGE
02063         KMETH = 1
02064         PRINT*,'AVERAGES OR LOCAL APERTURE:  1 = AVE  2 = LOC ?',KMETH
02065         READ*,KMETH
02066         IGEO = 2
02067         PRINT*,'INPUT IGEO',IGEO
02068         READ*,IGEO
02069         IOK = 0
02070         PRINT*,'INPUT OK',IOK
02071         READ*,IOK
02072         IF (IOK.EQ.0) GO TO 1620
02073   C
02074   C---  INITIALIZE PRESSURES  ---
02075   C
02076         IF (IPRINI .NE. 0) THEN
02077           DO 440 IDN = 1,NNOD
02078             THET = XNOD(IDN) /XMAX
02079             IF (IDBIN .NE. IDBEV) THET = YNOD(IDN) /YMAX
02080             IF ((IDBIN.EQ.2) .OR. (IDBIN.EQ.3)) THET = 1. - THET
02081             PRES(IDN) = PIN
02082             IF (ICOMP.EQ.0) THEN
02083               PRES(IDN) = PIN - (PIN-PEX)*THET
02084               IF (IPRINI .LT. 0.) PRES(IDN) = PEX
```

```
02085              ELSE
02086                PRES(IDN) = SQRT (PIN**2 - (PIN**2-PEX**2)*THET)
02087                IF (IPRINI .LT. 0.) PRES(IDN) = PEX
02088              ENDIF
02089              PRESO(IDN) = PRES(IDN)
02090    440     CONTINUE
02091          ENDIF
02092    C
02093          TIM = 0.
02094          DTIM = 0.1
02095          ISTOP = 0
02096          KMAX = 1
02097          TOUT = 0
02098    C
02099    C---  UPDATE CURRENT VALUES OF PRESSURE ---
02100    C
02101            DO 710 K = 1, KMAX
02102            IF (ISTOP.EQ.1) GO TO 830
02103            TIM = TIM + DTIM
02104            IF (K.GT.1) THEN
02105              DO 321 IDN = 1, NNOD
02106                PRINT*,IDN,PRESO(IDN)
02107    321         PRES(IDN) = PRESO(IDN)
02108            ENDIF
02109    C

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02110     1630   IGO = 0
02111    C
02112    C---  COMPUTE SPECIFIC SURFACE AREA  ---
02113    C
02114           SUMA = 0.
02115           SUMV = 0.
02116           DO 312 ID = 1, NPAR
02117             IF (IGEO .EQ. 2) THEN
02118               SUMA = SUMA + PI *DIAM(ID)
02119               SUMV = SUMV + PI *DIAM(ID)**2 /4.
02120             ELSE
02121               SUMA = SUMA + PI *DIAM(ID)**2
02122               SUMV = SUMV + PI *DIAM(ID)**3 /6.
02123             ENDIF
02124    312    CONTINUE
02125           SV000 = SUMA /SUMV
02126    C
02127    C---  COMPUTE EFFECTIVE PORE RADII  ---
02128    C
02129           PORSUM = 0.
02130           DO 317 IDN = 1, NNOD
02131             APORE(IDN) = 0.
02132             DO 316 J = 1, NODAR(1,IDN)
02133               IDT = NODAR (4+J, IDN)
02134               ID = TUBNOD (3, IDT)
02135               IDP = TUBNOD (4, IDT)
02136               IF (ID.GT.0 .AND. IDP.GT.0 ) THEN
02137                 BASE2 = (XS(ID)-XS(IDP))**2 + (YS(ID)-YS(IDP))**2
02138                 BASE = SQRT (BASE2)
02139                 RLEG = BASE /2.
02140                 XMID = (XS(ID) + XS(IDP)) /2.
02141                 YMID = (YS(ID) + YS(IDP)) /2.
02142                 HIGHT2 = (XNOD(IDN)-XMID)**2 + (YNOD(IDN)-YMID)**2
```

```
02143                 HIGHT = SQRT (HIGHT2)
02144                 DTHETA = ATAN (HIGHT /RLEG)
02145                 IF (RADI(ID)+RADI(IDP) .LE. BASE) THEN
02146                   APART = DTHETA /2. *(RADI(ID)**2 + RADI(IDP)**2)
02147                 ELSE
02148                   RLAP = (RADI(ID) + RADI(IDP) - BASE) /2.
02149                   PHI1 = ACOS ((RADI(ID)-RLAP) /RADI(ID))
02150                   HLAP = RADI(ID) *SIN (PHI1)
02151                   PHI2 = ACOS ((RADI(IDP)-RLAP) /RADI(IDP))
02152                   ATRI = (RADI(ID)-RLAP) *HLAP /2.
02153                   APART = (DTHETA-PHI1) /2. *RADI(ID)**2 + ATRI
02154                   ATRI = (RADI(IDP)-RLAP) *HLAP /2.
02155                   APART = APART + (DTHETA-PHI2)/2. *RADI(IDP)**2 + ATRI
02156                 ENDIF
02157                 DAREA = MAX (0., HIGHT *RLEG - APART)
02158               ELSE
02159                 IDSAV = ID
02160                 ID = MAX (ID, IDP)
02161                 IDP = MIN (IDSAV, IDP)
02162                 HYPOT2 = (XS(ID)-XNOD(IDN))**2 + (YS(ID)-YNOD(IDN))**2
02163                 HYPOT = MAX (1.E-10*XMAX, SQRT (HYPOT2))
02164                 IF (IDP/2*2 .EQ. IDP) THEN
02165                   RLEG = ABS (YS(ID) - YNOD(IDN))
02166                 ELSE

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02167                   RLEG = ABS (XS(ID) - XNOD(IDN))
02168                 ENDIF
02169                 HIGHT = SQRT (HYPOT2 - RLEG**2)
02170                 DTHETA = PI /2. - ACOS (RLEG /HYPOT)
02171                 IF (RADI(ID) .LE. HIGHT) THEN
02172                   APART = DTHETA /2. *RADI(ID)**2
02173                 ELSE
02174                   RLAP = RADI(ID) - HIGHT
02175                   PHI = ACOS ((RADI(ID)-RLAP) /RADI(ID))
02176                   HLAP = RADI(ID) *SIN (PHI)
02177                   ATRI = (RADI(ID)-RLAP) *HLAP /2.
02178                   APART = (DTHET-PHI) /2. *RADI(ID)**2 + ATRI
02179                 ENDIF
02180                 DAREA = MAX (0., HIGHT *RLEG /2. - APART)
02181               ENDIF
02182               APORE(IDN) = APORE(IDN) + DAREA
02183    316      CONTINUE
02184             PORSUM = PORSUM + APORE(IDN)
02185    317    CONTINUE
02186           EPSVOID = PORSUM /(XMAX*YMAX)
02187   C
02188   C---  COMPUTE MAX NODE DIAMETERS  ---
02189   C
02190           DO 318 IDN = 1, NNOD
02191             XTU(IDN) = XNOD(IDN)
02192             YTU(IDN) = YNOD(IDN)
02193             RTU(IDN) = XMAX /100.
02194             RMIN = XMAX
02195             DO 319 J = 1, NODAR(1,IDN)
02196               IDT = NODAR (4+J, IDN)
02197               ID = TUBNOD (3, IDT)
02198               IDP = TUBNOD (4, IDT)
02199               IF (ID.GT.0 .AND. IDP.GT.0 ) THEN
02200                 XAA(J,1) = -2. *(XS(ID) - XS(IDP))
```

```
02201                 XAA(J,2) = -2. *(YS(ID) - YS(IDP))
02202                 XAA(J,3) = -2. *(RADI(ID) - RADI(IDP))
02203                 RHS(J) = RADI(ID)**2 - RADI(IDP)**2
02204        1           - XS(ID)**2 + XS(IDP)**2 - YS(ID)**2 + YS(IDP)**2
02205                 QHS(J) = RADI(ID) - RADI(IDP)
02206                 DIS = SQRT ((XS(ID)-XS(IDP))**2 + (YS(ID)-YS(IDP))**2)
02207                 RTRY = DIS - RADI(ID) - RADI(IDP)
02208                 RMIN = MIN (RMIN, RTRY)
02209               ELSE
02210                 XAA(J,1) = 0.
02211                 XAA(J,2) = 0.
02212                 XAA(J,3) = 0.
02213                 RHS(J) = 0.
02214                 QHS(J) = 0.
02215                 IDSAV = ID
02216                 ID = MAX (ID, IDP)
02217                 IDP = MIN (IDSAV, IDP)
02218                 IF (IDP .EQ. -2 .OR. IDP .EQ. -4) THEN
02219                   XAA(J,1) = 1.
02220                   RHS(J) = 0.
02221                   IF (IDP .EQ. -2) RHS(J) = XMAX
02222                 ELSE
02223                   XAA(J,2) = 1.

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02224                   RHS(J) = 0.
02225                   IF (IDP .EQ. -3) RHS(J) = YMAX
02226                 ENDIF
02227               ENDIF
02228    319      CONTINUE
02229    C
02230             WT = 1.
02231             WTR = 0.3
02232             RTU(IDN) = 1.1 *RMIN
02233             RNEW = RTU(IDN)
02234             ITSK = 0
02235             DO 377 ITS = 1, 50
02236               ITSK = ITSK + 1
02237    C
02238               RTU(IDN) = (1.-WTR) *RTU(IDN) + WTR *RNEW
02239               DETA = XAA(1,1) *XAA(2,2) - XAA(1,2) *XAA(2,1)
02240               XHS(1) = RHS(1) + 2.* QHS(1) *RTU(IDN)
02241               XHS(2) = RHS(2) + 2.* QHS(2) *RTU(IDN)
02242               DETX = XHS(1)   *XAA(2,2) - XAA(1,2) *XHS(2)
02243               DETY = XAA(1,1) *XHS(2)   - XHS(1)   *XAA(2,1)
02244               XNEW = DETX /DETA
02245               YNEW = DETY /DETA
02246               XTU(IDN) = (1.-WT) *XTU(IDN) + WT *XNEW
02247               YTU(IDN) = (1.-WT) *YTU(IDN) + WT *YNEW
02248    C
02249               DELM = 0.
02250               ERR = 0.
02251               DO 376 J = 1, NODAR(1,IDN)
02252                 ID = NODAR(J+8,IDN)
02253                 IF (ID .LT. 1) GO TO 376
02254                 RTUF = (XS(ID)-XTU(IDN))**2 + (YS(ID)-YTU(IDN))**2
02255                 RXX = SQRT (RTUF) - RADI(ID)
02256                 RES(J) = SQRT(RTUF) - RADI(ID) - RTU(IDN)
02257                 ERR = MAX (ERR, ABS(RES(J)))
02258                 IF (ABS(RXX-RTU(IDN)) .GT. DELM) THEN
```

```
02259                   DELM = ABS (RXX-RTU(IDN))
02260                   RNEW = RXX
02261                 ENDIF
02262    376        CONTINUE
02263               IF (ERR .LT. 1.E-6*XMAX) GO TO 378
02264    C
02265     377      CONTINUE
02266     378      CONTINUE
02267              RTU(IDN) = MAX (RTU(IDN), 1.E-30)
02268    C
02269     318    CONTINUE
02270    C
02271    C---   COMPUTE EFFECTIVE TUBE DIAMETERS FOR 3-D GEOMETRY
02272    C
02273           IF (IGEO .EQ. 3) THEN
02274             BBAR = 0.
02275             MSUM = 0
02276             ELBAR = 0.
02277             DO 344 IDT = 1, NTUB
02278               IDN = TUBNOD(1,IDT)
02279               IDNP = TUBNOD(2,IDT)
02280               AR1 =  PI *RTU(IDN)**2

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02281               AR2 =  PI *RTU(IDNP)**2
02282               AR1 = MAX (AR1, 1.E-20)
02283               AR2 = MAX (AR2, 1.E-20)
02284               TUL = TUBAR(1,IDT)
02285               TUL1 = TUL /2.
02286               TUL2 = TUL /2.
02287               AEFF = (TUL1 *AR1 + TUL2 *AR2) /TUL
02288               RAD1 = SQRT (AR1 /PI)
02289               RAD2 = SQRT (AR2 /PI)
02290               RK1 = MAX (RAD1**2 /8., 1.E-20)
02291               RK2 = MAX (RAD2**2 /8., 1.E-20)
02292               IF (RK1 .LT. RK2) THEN
02293                 BOT = AEFF /TUL *(TUL1 /AR1 + TUL2 *RK1 /RK2 /AR2)
02294                 RKEFF = RK1 /BOT
02295               ELSE
02296                 BOT = AEFF /TUL *(TUL1 *RK2 /RK1 /AR1 + TUL2 /AR2)
02297                 RKEFF = RK2 /BOT
02298               ENDIF
02299               RKEFF = MAX (RKEFF, 1.E-30)
02300               DEFF = SQRT (32. *RKEFF)
02301               DPER(IDT) = SQRT (12. *RKEFF)
02302               DVOL(IDT) = AEFF
02303               DDIF(IDT) = TUL /(TUL1 /AR1 + TUL2 /AR2)
02304               TUBAR(14,IDT) = 2. *SQRT (AEFF /PI)
02305               TUBAR(15,IDT) = DDIF(IDT)
02306               IF (TUBAR(9,IDT) .LT. 0) THEN
02307                 DPER(IDT) = 0.
02308                 DVOL(IDT) = 0.
02309                 DDIF(IDT) = 0.
02310                 TUBAR(14,IDT) = 0.
02311                 TUBAR(15,IDT) = 0.
02312               ENDIF
02313               IF (TUBAR(9,IDT) .GT. 0) THEN
02314                 MSUM = MSUM + 1
02315                 BBAR = BBAR + TUBAR(14,IDT)
02316                 ELBAR = ELBAR + TUBAR(1,IDT)
```

```
02317                ENDIF
02318     344      CONTINUE
02319              BBAR = BBAR /MSUM
02320              ELBAR = ELBAR /MSUM
02321            ELSE
02322   C
02323   C---  COMPUTE CHARACTERISTIC 2-D PASSAGE DIMENSIONS  ---
02324   C
02325              IPIK = 1
02326              BBAR = 0.
02327              MSUM = 0
02328              ELBAR = 0.
02329              DO 371 IDT = 1, NTUB
02330                ID = TUBNOD(3,IDT)
02331                IDP = TUBNOD(4,IDT)
02332                IF (ID.GT.0 .AND. IDP.GT.0) THEN
02333                  R1 = RADI(ID)
02334                  R2 = RADI(IDP)
02335                ELSE
02336                  ID = MAX (ID, IDP)
02337                  R1 = RADI(ID)

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02338                  R2 = R1
02339                ENDIF
02340                DNEK = TUBAR(2,IDT)
02341                RLEN = MIN (MIN (TUBAR(1,IDT), 1.999*R1), 1.999*R2)
02342                CALL DELTAS (IPIK, R1, R2, DNEK, RLEN, DDIF(IDT),
02343         1                   DPER(IDT), DVOL(IDT))
02344                TUBAR(14,IDT) = DVOL(IDT)
02345                TUBAR(15,IDT) = DDIF(IDT)
02346                IF (TUBAR(9,IDT) .GT. 0) THEN
02347                  MSUM = MSUM + 1
02348                  BBAR = BBAR + DVOL(IDT)
02349                  ELBAR = ELBAR + TUBAR(1,IDT)
02350                ENDIF
02351     371      CONTINUE
02352              BBAR = BBAR /MSUM
02353              ELBAR = ELBAR /MSUM
02354            ENDIF
02355   C
02356   C---  CYCLE OVER RELAXATION STEPS  ---
02357   C
02358            ICONV = 1
02359            DO 210 ICY = 1,NSOR
02360              IGO = IGO + 1
02361              ERR = 0.
02362              ERRMDT = 0.
02363   C
02364   C---  COMPUTE MASS FLOW RATES AND WEIGHTS FOR EACH NODE.
02365   C     SIGN CONVENTION FOR FLOW IS POSITIVE FOR POSITIVE FLOW FROM
02366   C     NODE N1 TO NODE N2;  PRESSURE GRADIENT IS (P2-P1)/L.
02367   C
02368              DO 220 IDN = 1,NNOD
02369                VOL = 0.
02370                DOTM = 0.
02371                WGTSUM = 0.
02372                DPDRHO = 1.
02373                IF (ICOMP.EQ.1) DPDRHO = RGAS *TMP
02374                DO 230 L = 1, NODAR(1,IDN)
```

```
02375                 NUM = NODAR(L+1,IDN)
02376                 IDT = NODAR(L+4,IDN)
02377                 N1 = TUBNOD(1,IDT)
02378                 TUL = TUBAR(1,IDT)
02379                 TUD = TUBAR(2,IDT)
02380                 ALF = DPER(IDT)**2 /12.
02381                 VOL = VOL + DVOL(IDT) *TUL /2.
02382                 PBAR = (PRES(IDN)+PRES(NUM))/2.
02383                 RHO = 1.
02384                 IF (ICOMP.EQ.1) RHO = PBAR /RGAS /TMP
02385                 RMU = 1.
02386                 DPDL = (PRES(IDN)-PRES(NUM)) /TUL
02387                 VEL = - ALF /RMU *DPDL
02388                 DOTM = DOTM + VEL *RHO *DVOL(IDT)
02389                 WGTSUM = WGTSUM + ALF/RMU/TUL *RHO *DVOL(IDT)
02390                 ISGN = 1
02391                 IF (NUM .NE. N1) ISGN = - 1
02392                 TUBAR(10,IDT) = ISGN *VEL
02393                 TUBAR(11,IDT) = ISGN *VEL *RHO *DVOL(IDT)
02394                 TUBAR(12,IDT) = DVOL(IDT) *TUL

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02395                 TUBAR(13,IDT) = ISGN *VEL *DVOL(IDT)
02396    230        CONTINUE
02397   C
02398   C---  COMPUTE RESIDUAL OF GOVERNING EQUATION FOR NODE IDN  ---
02399   C
02400               IF (NODAR(8,IDN).EQ.-IDBIN .OR. NODAR(8,IDN).EQ.-IDBOU) THEN
02401                 DPRES(IDN) = 0.
02402               ELSE
02403                 PDOT = (PRES(IDN)-PRESO(IDN)) /DTIM
02404                 RESP = 0.0000000 *PDOT - DOTM /VOL *DPDRHO
02405                 WEIGHT = WGT *VOL /DPDRHO /WGTSUM
02406                 DPRES(IDN) = - WEIGHT *RESP
02407               ENDIF
02408   C
02409   C---  UPDATE PRESSURES AND NODE IDN  ---
02410   C
02411               PRES(IDN) = PRES(IDN) + DPRES(IDN)
02412               IF (NODAR(8,IDN) .EQ. -IDBIN) PRES(IDN) = PIN
02413               IF (NODAR(8,IDN) .EQ. -IDBOU) PRES(IDN) = PEX
02414   C
02415   C---  COMPUTE LOCAL ERROR ESTIMATE AT NODE IDN  ---
02416   C
02417               TOL = RELERR *ABS(PIN-PEX) *WGT
02418               ERRIDN = ABS(DPRES(IDN)) /TOL
02419               IF (ERRIDN .GT. ERR) THEN
02420                 ERR = ERRIDN
02421                 IDNERR = IDN
02422               ENDIF
02423   C
02424   C---  NOTE MAXIMUM NET FLOW RATE AT INTERIOR POINTS
02425   C
02426               IF ((NODAR(8,IDN).NE.-IDBIN) .AND.
02427         1          (NODAR(8,IDN).NE.-IDBOU)) THEN
02428                 IF (ABS(DOTM) .GT. ERRMDT) THEN
02429                   ERRMDT = ABS(DOTM)
02430                   IDNMDT = IDN
02431                 ENDIF
02432               ENDIF
```

```
02433   C
02434    220      CONTINUE
02435             IF (ERR.LT.1.0) GO TO 280
02436   C
02437   C---  PRINT CURRENT MAXIMUM ERROR, NODE IDENTIFIERS AND PRESSURES  ---
02438   C
02439             IF (MOD(IGO,100).EQ.0) THEN
02440               PRINT903,IGO,IDNERR,NODAR(8,IDNERR),ERRMDT,
02441        1           ERR,PRES(IDNERR),XNOD(IDNERR),YNOD(IDNERR)
02442             ENDIF
02443   C
02444    210    CONTINUE
02445           ICONV = 0
02446    280    CONTINUE
02447   C
02448   C---  SUM FLOW RATES AND POROSITY
02449   C
02450           DOTMIN = 0.
02451           DOTMOUT = 0.

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02452           SUMDOT = 0.
02453           DO 892 IDT = 1, NTUB
02454   C
02455             N1 = TUBNOD(1,IDT)
02456             N2 = TUBNOD(2,IDT)
02457             IF (NODAR(8,N1) .EQ. NODAR(8,N2)) GO TO 892
02458   C
02459   C---  GLOBAL MASS BALANCE FOR ALL INTERIOR NODES
02460   C     TUBE MUST HAVE ONE BOUNDARY ( < 0 ) AND ONE INTERIOR ( = 0 ) NODE
02461   C
02462             IF (NODAR(8,N1)*NODAR(8,N2) .EQ. 0) THEN
02463               NN = MIN (NODAR(8,N1), NODAR(8,N2))
02464               NEVEN = (NN /2) *2
02465               ISNN = 1
02466               IF ((XNOD(N1).GT.XNOD(N2)) .AND. (NN.EQ.NEVEN)) ISNN = - 1
02467               IF ((YNOD(N1).GT.YNOD(N2)) .AND. (NN.NE.NEVEN)) ISNN = - 1
02468               SUMDOT = SUMDOT + ISNN *NORM(-NN) *TUBAR(11,IDT)
02469             ENDIF
02470   C
02471   C---  SUM MASS FLOW RATES INTO AND OUT OF X = 0 AND X = L
02472   C
02473             ISNX = 1
02474             IF (IDBIN .EQ. IDBEV) THEN
02475               IF (XNOD(N1) .GT. XNOD(N2)) ISNX = - 1
02476             ELSE
02477               IF (YNOD(N1) .GT. YNOD(N2)) ISNX = - 1
02478             ENDIF
02479   C
02480             IF     (NODAR(8,N1).EQ.-IDBOU .OR. NODAR(8,N2).EQ.-IDBOU) THEN
02481               DOTMOUT = DOTMOUT + ISNX *TUBAR(11,IDT)
02482             ELSEIF (NODAR(8,N1).EQ.-IDBIN .OR. NODAR(8,N2).EQ.-IDBIN) THEN
02483               DOTMIN = DOTMIN + ISNX *TUBAR(11,IDT)
02484             ENDIF
02485   C
02486    892    CONTINUE
02487   C
02488           PBAR = (PIN + PEX) /2.
02489           RHO = 1.
02490           IF (ICOMP.EQ.1) RHO = PBAR /RGAS /TMP
```

```
02491           RMU = 1.
02492           UBAR = (ABS(DOTMIN)+ABS(DOTMOUT))/2. /YMAX /RHO
02493           IF (IGEO .EQ. 3) UBAR = UBAR /ELBAR
02494           VBAR = UBAR /PORO
02495   C---  OLD UREF WAS UBAR  ---
02496           UREF = VBAR
02497           PERM = UBAR *RMU *XMAX /ABS(PIN-PEX)
02498           SV0 = 4. /DREF
02499           IF (IGEO .EQ. 3) SV0 = 6. /DREF
02500           PERM0 = EPSVOID**3 /(1.-EPSVOID)**2 /SV0**2
02501           PERM0 = EPSMC**3 /(1.-EPSMC)**2 /SV0**2
02502           RKOZE = PERM0 /PERM
02503           TAU0 = DIAMF**2 *PI /2. /(1.-PORO)
02504           EDSK = PERM /TAU0
02505           PRINT900,UBAR,VBAR
02506           PRINT900,(TUBAR(10,IT),IT=1,10)
02507           PRINT900,(TUBAR(10,IT+NTUB/2),IT=1,10)
02508   C

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02509           SUMV = 0.
02510           SUMW = 0.
02511           DO 819 IDT = 1, NTUB
02512             VOLT = TUBAR(1,IDT) *DVOL(IDT)
02513             SUMV = SUMV + VOLT
02514             SUMW = SUMW + ABS(TUBAR(10,IDT)) *VOLT
02515    819    CONTINUE
02516           VAVE = SUMW /SUMV
02517           RHOS = 1. - SUMV /XMAX /YMAX
02518           PRINT900, VAVE, RHOS
02519   C
02520           PRINT900,SUMDOT,DOTMIN,DOTMOUT,PERM,RKOZE
02521   C
02522   C---  SOLICIT INPUT FOR CONTINUATION  ---
02523   C
02524           PRINT*,'INPUT ICONT 1 = MORE CYCL  2 = NEW PRESS
02525         1    3 = NEW TUBES  4 = RESTART'
02526           READ*,ICONT
02527           IF (ICONT.EQ.1) THEN
02528             PRINT*,'INPUT NSOR, WGT',NSOR,WGT
02529             READ*,NSOR,WGT
02530             GO TO 1630
02531           ELSEIF (ICONT.EQ.2) THEN
02532             GO TO 1620
02533           ELSEIF (ICONT.EQ.4) THEN
02534             GO TO 1600
02535           ENDIF
02536   C
02537   C     ADJUST TIME STEP
02538   C
02539           DO 832 IDT = 1, 0 *NTUB
02540             N1 = TUBNOD(1,IDT)
02541             N2 = TUBNOD(2,IDT)
02542             TUL = TUBAR(1,IDT)
02543             TUD = TUBAR(2,IDT)
02544             DOTM = TUBAR(11,IDT)
02545             IF (NODAR(8,N1) .EQ. NODAR(8,N2)) GO TO 832
02546             IF      (NODAR(8,N1).LT.0 .OR. NODAR(8,N2).LT.0) THEN
02547               PRINT903,IDT,NODAR(8,N1),NODAR(8,N2),DOTM,TUBAR(3,IDT),
02548         1       TUBAR(4,IDT),TUBAR(5,IDT),TUBAR(6,IDT),PRES(N1),PRES(N2)
```

```
02549              ENDIF
02550    C
02551     832     CONTINUE
02552             DO 833 IDT = 1, 0 *NTUB
02553               N1 = TUBNOD(1,IDT)
02554               N2 = TUBNOD(2,IDT)
02555               TUL = TUBAR(1,IDT)
02556               TUD = TUBAR(2,IDT)
02557               DOTM = TUBAR(11,IDT)
02558               IF (NODAR(8,N1) .NE. NODAR(8,N2)) GO TO 833
02559               IF      (NODAR(8,N1).LT.0 .OR. NODAR(8,N2).LT.0) THEN
02560                 PRINT903,IDT,NODAR(8,N1),NODAR(8,N2),DOTM,TUBAR(3,IDT),
02561         1       TUBAR(4,IDT),TUBAR(5,IDT),TUBAR(6,IDT),PRES(N1),PRES(N2)
02562               ENDIF
02563     833     CONTINUE
02564    C
02565    C      PLOTT PRESSURE POINTS

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02566    C
02567             IF (IPLTPR.EQ.1) THEN
02568               CALL AREA2D(XAXIS,YAXIS)
02569               CALL GRAF(XORIG,XSTP,XMAX,YORIG,YSTP,YMAX)
02570               CALL THKFRM(.030)
02571               CALL FRAME
02572               PRINT*,ISEED0
02573               PRINT913,NPAR
02574               PRINT913,NNOD
02575               PRINT913,NTUB
02576               PRINT913,NSOR
02577               PRINT900,PIN
02578               PRINT900,PEX
02579               PRINT900,PORO
02580               PRINT900,ABSERR
02581               PRINT900,RELERR
02582               PRINT900,WGT
02583               PRINT*,' '
02584               IF (ICONV.EQ.0) PRINT*,'NO SOR CONV'
02585               PRINT*,IGO
02586               PRINT900,ERR
02587               PRINT900,DOTMIN
02588               PRINT900,DOTMOUT
02589               PRINT900,DOTMUP
02590               PRINT900,DOTMDN
02591               CALL MARKER(15)
02592               DO 827 IDN = 1,NNOD
02593                  XB(1)=XNOD(IDN)
02594                  YB(1)=YNOD(IDN)
02595                  FAC = (PRES(IDN)-PEX) /(PIN-PEX)
02596                  FAC = FAC/SQRT(1.*NNOD) *XAXIS/0.082
02597                  CALL SCLPIC(FAC)
02598                  CALL CURVE(XB,YB,1,1)
02599    827           CONTINUE
02600               CALL SCLPIC(1.)
02601               CALL ENDPL(0)
02602             ENDIF
02603    C
02604    C      PLOTT X-P PRESSURE PROFILE
02605    C
02606             XORIG = 0.
```

```
02607           YORIG = 0.
02608           YMAX2 = 1.
02609           CALL SCLPIC(1.)
02610           IF (IPLTPF.EQ.1) THEN
02611             IF (RATXY.GT.1.0) THEN
02612               XAXIS = 7.5
02613               YAXIS = 0.95775 *7.5
02614             ELSE
02615               XAXIS = 7.5 *RATXY
02616               YAXIS = 0.95775 *7.5
02617             ENDIF
02618             XSTP=(XMAX-XORIG)/1.
02619             YSTP=(YMAX2-YORIG)/1.
02620             CALL AREA2D(XAXIS,YAXIS)
02621             CALL GRAF(XORIG,XSTP,XMAX,YORIG,YSTP,YMAX2)
02622             CALL FRAME

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02623             CALL MARKER(15)
02624             PRINT*,ISEED0
02625             PRINT913,NPAR
02626             PRINT913,NNOD
02627             PRINT913,NTUB
02628             PRINT913,NSOR
02629             PRINT900,PIN
02630             PRINT900,PEX
02631             PRINT900,PORO
02632             PRINT900,ABSERR
02633             PRINT900,RELERR
02634             PRINT900,WGT
02635             PRINT*,' '
02636             IF (ICONV.EQ.0) PRINT*,'NO SOR CONV'
02637             PRINT901,IGO
02638             PRINT900,ERR
02639             PRINT900,DOTMIN
02640             PRINT900,DOTMOUT
02641             PRINT900,SUMDOT
02642             DO 826 IDN = 1,NNOD
02643               XB(1) = XNOD(IDN)
02644               YB(1) = (PRES(IDN)-PEX) /(PIN-PEX)
02645               CALL CURVE(XB,YB,1,1)
02646   826       CONTINUE
02647             IF (IDBIN .EQ. IDBEV) THEN
02648               JMX = 200
02649               DO 825 J = 1, JMX
02650                 XB(J) = XMAX *(J-1.)/(JMX-1.)
02651                 IF (IDBIN .EQ. 2) XB(J) = 1. - XB(J)
02652                 IF (ICOMP.EQ.0) THEN
02653                   YB(J) = 1. - XB(J)/XMAX
02654                 ELSE
02655                   YB(J) = SQRT (PIN**2 - (PIN**2-PEX**2)*XB(J)/XMAX)
02656                   YB(J) = (YB(J)-PEX) /(PIN-PEX)
02657                 ENDIF
02658    825        CONTINUE
02659               CALL CURVE(XB,YB,JMX,0)
02660             ENDIF
02661   C
02662   C---  PLOT TUBE CONNECTIONS IN X-P SPACE  ---
02663   C
02664             CALL DASH
```

```
02665              DO 828 IDT = 1, NTUB
02666                IF (KBLOC(IDT) .EQ. 1) THEN
02667                  DO 829 J = 1, 2
02668                    IDN = TUBNOD(J,IDT)
02669                    XB(J) = XNOD(IDN)
02670     829            YB(J) = (PRES(IDN)-PEX) /(PIN-PEX)
02671                  CALL CURVE (XB,YB,2,0)
02672                ENDIF
02673     828        CONTINUE
02674                CALL RESET('DASH')
02675                CALL ENDPL(0)
02676              ENDIF
02677    C
02678    C       PLOTT Y-P PRESSURE PROFILE
02679    C

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02680              XORIG = 0.
02681              YORIG = 0.
02682              YMAX2 = 1.
02683              IF (IPLTPFY .EQ. 1) THEN
02684                IF (RATXY.GT.1.0) THEN
02685                  XAXIS = 7.5
02686                  YAXIS = 0.95775 *7.5
02687                ELSE
02688                  XAXIS = 7.5 *RATXY
02689                  YAXIS = 0.95775 *7.5
02690                ENDIF
02691                XSTP=(XMAX-XORIG)/1.
02692                YSTP=(YMAX2-YORIG)/1.
02693                CALL AREA2D(XAXIS,YAXIS)
02694                CALL GRAF(XORIG,XSTP,XMAX,YORIG,YSTP,YMAX2)
02695                CALL FRAME
02696                CALL MARKER(15)
02697                PRINT*,ISEED0
02698                PRINT913,NPAR
02699                PRINT913,NNOD
02700                PRINT913,NTUB
02701                PRINT913,NSOR
02702                PRINT900,PIN
02703                PRINT900,PEX
02704                PRINT900,PORO
02705                PRINT900,ABSERR
02706                PRINT900,RELERR
02707                PRINT900,WGT
02708                PRINT*,' '
02709                IF (ICONV.EQ.0) PRINT*,'NO SOR CONV'
02710                PRINT901,IGO
02711                PRINT900,ERR
02712                PRINT900,DOTMIN
02713                PRINT900,DOTMOUT
02714                PRINT900,SUMDOT
02715                DO 856 IDN = 1,NNOD
02716                  XB(1) = YNOD(IDN)
02717                  YB(1) = (PRES(IDN)-PEX) /(PIN-PEX)
02718                  CALL CURVE(XB,YB,1,1)
02719     856        CONTINUE
02720                IF (IDBIN .NE. IDBEV) THEN
02721                  JMX = 200
02722                  DO 855 J = 1, JMX
```

```
02723                 XB(J) = YMAX *(J-1.)/(JMX-1.)
02724                 IF (IDBIN .EQ. 3) XB(J) = 1. - XB(J)/YMAX
02725                 IF (ICOMP.EQ.0) THEN
02726                   YB(J) = 1. - XB(J)
02727                 ELSE
02728                   YB(J) = SQRT (PIN**2 - (PIN**2-PEX**2)*XB(J)/YMAX)
02729                   YB(J) = (YB(J)-PEX) /(PIN-PEX)
02730                 ENDIF
02731    855        CONTINUE
02732               CALL CURVE(XB,YB,JMX,0)
02733             ENDIF
02734   C
02735   C---  PLOT TUBE CONNECTIONS IN Y-P SPACE  ---
02736   C

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02737             CALL DASH
02738             DO 858 IDT = 1, NTUB
02739               IF (KBLOC(IDT) .EQ. 1) THEN
02740                 DO 859 J = 1, 2
02741                   IDN = TUBNOD(J,IDT)
02742                   XB(J) = YNOD(IDN)
02743    859            YB(J) = (PRES(IDN)-PEX) /(PIN-PEX)
02744                 CALL CURVE (XB,YB,2,0)
02745               ENDIF
02746    858      CONTINUE
02747             CALL RESET('DASH')
02748             CALL ENDPL(0)
02749           ENDIF
02750   C
02751   C     UPDATE VALUES
02752   C
02753           DO 740 ID=1,IDMX
02754             PRESO(IDN) = PRES(IDN)
02755    740    CONTINUE
02756   C
02757   C--- WRITE RESTART FILE  ---
02758   C
02759         IFILE = 99
02760         PRINT*,'INPUT FILE NUMBER FOR WRITING RESTART FILE',IFILE
02761         READ*,IFILE
02762         IF (IFILE .GT. 0) THEN
02763           REWIND (IFILE)
02764           WRITE(IFILE,922) NSEED,ISEED0,XMAX,YMAX,PORO,SPAC,SPACM,TOL,
02765        1                   EPS0,DIAMF,PIN,PEX
02766           DO 414 I = 1, NSEED
02767    414      WRITE(IFILE,*) XS(I),YS(I),HITE(I),DIAM(I),RADI(I)
02768           WRITE(IFILE,901) NNOD
02769           DO 415 I = 1, NNOD
02770    415      WRITE(IFILE,*) PRES(I)
02771         ENDIF
02772   C
02773   C---  TRACER PARTICLE MOTION  ---
02774   C
02775         IF (KPAR .GT. 0) THEN
02776           XORIG=0.
02777           YORIG=0.
02778           RATXY=XMAX/YMAX
02779           IF (RATXY.GT.1.0) THEN
02780             XAXIS = 7.5
```

```
02781             YAXIS=XAXIS *0.95775 /RATXY
02782           ELSE
02783             XAXIS = 7.5 *RATXY
02784             YAXIS=XAXIS *0.95775 /RATXY
02785           ENDIF
02786           XSTP=(XMAX-XORIG)/1.
02787           YSTP=(YMAX-YORIG)/1.
02788           CALL AREA2D(XAXIS,YAXIS)
02789           CALL GRAF(XORIG,XSTP,XMAX,YORIG,YSTP,YMAX)
02790           CALL FRAME
02791    C
02792           DCOF = ABS (UREF *DIAMF/1.000 /PECL)
02793           PECS = PECL *SDEVT /DTBAR

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02794           DTIM1 = ABS (XMAX /VBAR *DTSTR)
02795           DTIM2 = (XMAX *DTSTR)**2 /DCOF /2.
02796           DTIM = 1. /(1./DTIM1 + 1./DTIM2)
02797           DTIM = DTIM1
02798    C
02799           PRINT981,'METH',IMETH
02800           PRINT980,'DIAM',DIAMF
02801           PRINT980,'DREF',DREF
02802           PRINT980,'UBAR',UBAR
02803           PRINT980,'UREF',UREF
02804           PRINT980,'VBAR',VBAR
02805           PRINT980,'VAVE',VAVE
02806           PRINT980,'PERM',PERM
02807           PRINT980,'SV00',SV000
02808           PRINT980,'RKOZ',RKOZE
02809           PRINT980,'EDSK',EDSK
02810           PRINT980,'EPS0',EPS0
02811           PRINT980,'PORO',PORO
02812           PRINT980,'EPSV',EPSVOID
02813           PRINT980,'EPSM',EPSMC
02814           PRINT980,'RHOS',RHOS
02815           PRINT980,'DTIM',DTIM
02816           PRINT980,'DTST',DTSTR
02817           PRINT980,'DCOF',DCOF
02818           PRINT980,'PECL',PECL
02819           PRINT980,'PECS',PECS
02820           PRINT980,'TBAR',DTBAR
02821           PRINT980,'BBAR',BBAR
02822           PRINT980,'TSIG',SDEVT
02823           TSTAR = DCOF *DTIM /DTBAR**2
02824           PRINT980,'TSTR',TSTAR
02825           IF (TSTAR.LT.1.0) PRINT980,'TSTR TOO SMALL'
02826    C
02827           CALL MARKER(16)
02828           CALL BLREC(-0.2*XAXIS,-0.2*YAXIS,0.2*XAXIS,1.4*YAXIS,0)
02829           CALL BLREC(-0.2*XAXIS,-0.2*YAXIS,1.4*XAXIS,0.2*YAXIS,0)
02830           CALL BLREC( 1.0*XAXIS,-0.2*YAXIS,0.2*XAXIS,1.4*YAXIS,0)
02831           CALL BLREC(-0.2*XAXIS, 1.0*YAXIS,1.4*XAXIS,0.2*YAXIS,0)
02832           DO 1381 ID = 1, NSEED
02833             XB(1)=XS(ID)
02834             YB(1)=YS(ID)
02835             FAC= 2.* RADI(ID)/XMAX *XAXIS/0.082
02836             CALL SCLPIC(FAC)
02837             CALL CURVE(XB,YB,1,1)
02838    1381   CONTINUE
```

```
02839           CALL SCLPIC(1.)
02840           CALL RESET('BLSYM')
02841           CALL SCLPIC(1.0)
02842   C
02843           DO 1369 IFR = 1, 100
02844    1369     FREQ(IFR) = 0.
02845   C
02846           DO 1707 IDT = 1, NTUB
02847    1707     JBLOK(IDT) = 0
02848   C
02849           ASUM = 0.
02850           DO 1374 I = 1, NNBC(IDBIN)

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02851             IDN = NBID(IDBIN,I)
02852             IDT = TBID(IDBIN,I)
02853             ASUM = ASUM + KBLOC(IDT) *TUBAR(15,IDT)
02854    1374   CONTINUE
02855   C
02856           VTBAR = 0.
02857           XBAR = 0.
02858           KPSUM = 0
02859           TORSUM = 0.
02860           ARTBAR = 0.
02861           DO 1310 J = 1, KPAR
02862   C
02863   C---  GENERATE NEW PARTICLE AND PLACE AT ENTRANCE NODE; PARTICLES ARE
02864   C     RANDOMLY DISTRIBUTED BETWEEN ENTRANCE NODES IN PROPORTION TO
02865   C     INLET TUBE FLOW RATES.
02866   C
02867    1315     CONTINUE
02868             DPART = - 100 *SPACM /10.
02869             XXX = RAN(ISED)
02870             XTRM = (4.*XXX-2.)/3.
02871             ZZZ = XTRM
02872             DO 1382 I = 1, 100
02873               ZZZ = ZZZ**3 /3. + XTRM
02874               RESID = ZZZ**3 - 3.*ZZZ + 3.*XTRM
02875               IF (ABS(RESID) .LT. 1.E-4) GO TO 1383
02876    1382     CONTINUE
02877             WRITE(17,*) 'ZZZ DID NOT CONVERGE',XXX,ZZZ,RESID
02878    1383     CONTINUE
02879   C
02880   C--- OPTION FOR UNIFORM INJECTION  ---
02881   C
02882             IF (IUNI .EQ. 1) THEN
02883               ZZZ = (2.*XXX - 1.)
02884             ENDIF
02885   C
02886             GGG = (ZZZ + 1.) /2.
02887   C
02888   C---  SUM ENTRANCE FLOWS TO PICK INLET TUBE  ---
02889   C
02890             XXX = RAN(ISED)
02891             XXX = EDGE + (1.-2.*EDGE) *XXX
02892             IF (XXX0 .LT. 0.) THEN
02893               XXX = -XXX0
02894             ENDIF
02895             FLSUM = 0.
02896             DO 1364 I = 1, NNBC(IDBIN)
```

```
02897                IDN = NBID(IDBIN,I)
02898                IDT = TBID(IDBIN,I)
02899                DFLUX = ABS(TUBAR(11,IDT)) /DOTMIN
02900                DFLUX = DFLUX + 0.00000 *TUBAR(15,IDT) /ASUM /PECL
02901                FLSUM = FLSUM + DFLUX /(1. + 0.00000 /PECL)
02902                IF (FLSUM .GT. XXX) THEN
02903                  INOD = IDN
02904                  GO TO 1365
02905                ENDIF
02906     1364     CONTINUE
02907              WRITE(17,*) 'CANT FIND ENTRANCE NODE'

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02908     C
02909      1365     TREM = DTIM
02910              IDON = 0
02911              TORT = 0.
02912              XYNPAR(4,J) = YNOD(INOD)
02913              CALL THKCRV(.020)
02914     C
02915     C---  STEP THROUGH TUBE SET ALONG PARTICLE PATH  ---
02916     C
02917              DO 1320 ISTP = 1, 10000
02918                IF (IDON .EQ. 1) GO TO 1321
02919     C
02920     C---  IDENTIFY TUBES HAVING (POSITIVE) FLOW OUT OF NODE IDNOD
02921     C     AND SUM TUBE CROSS SECTION AREAS  ---
02922     C
02923                IF (ISTP .EQ. 1) GO TO 1363
02924                IDTIN = IDT
02925                DIFSUM = 0.
02926                FLOSUM = 0.
02927                NCH = NODAR(1,INOD)
02928                NFIN = 0
02929                NFOUT = 0
02930                DO 1330 JNOD = 1, NCH
02931                  IDT = NODAR(4+JNOD,INOD)
02932                  ADIF =  1.00000 *TUBAR(15,IDT)
02933                  QFLO = TUBAR(13,IDT)
02934                  DIFSUM = DIFSUM + ADIF *DCOF /TUBAR(1,IDT)
02935                  ISN = 1
02936                  IF (TUBNOD(1,IDT) .NE. INOD) ISN = -1
02937                  FLOW = ISN *QFLO
02938                  IF (FLOW .GT. 0.0) THEN
02939                    NFOUT = NFOUT + 1
02940                    FLOSUM = FLOSUM + FLOW
02941                    FLO(JNOD) = FLOW
02942                  ELSE
02943                    NFIN = NFIN + 1
02944                    FLO(JNOD) = 0.
02945                  ENDIF
02946     1330       CONTINUE
02947                FLOSUM = MAX (FLOSUM, 1.E-30)
02948                DIFSUM = MAX (DIFSUM, 1.E-30)
02949     C
02950     C---  IDENDITFY TUBE/NODE SEQUENCE NUMBER OF INFLOW TUBE  ---
02951     C
02952                QFLOIN = MIN (ABS (TUBAR(13,IDTIN)), FLOSUM) /FLOSUM
02953                DO 1398 JNOD = 1, NCH
02954                  IF (NODAR(4+JNOD,INOD) .EQ. IDTIN) THEN
```

```
02955                   JNODIN = JNOD
02956                   GO TO 1393
02957                 ENDIF
02958    1398       CONTINUE
02959    1393       CONTINUE
02960   C
02961   C---  MIX JUNCTION STREAMLINES  ---
02962   C
02963               IF (IMIX .EQ. 1) THEN
02964                 ZZZ = 2. *RAN(ISED) - 1.

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02965               ENDIF
02966   C
02967   C---  SELECT TUBE BASED ON RELATIVE FLUXES  ---
02968   C
02969               GGG = (ZZZ + 1.) /2.
02970               FLSUM = 0.
02971               DO 1335 JCNT = 1, NCH
02972                 JNOD = MOD (JNODIN+JCNT-1, NCH) + 1
02973                 IDTJ = NODAR(4+JNOD,INOD)
02974                 DFLOW = FLO(JNOD) /FLOSUM
02975                 FLSUM = FLSUM + DFLOW
02976                 IF (FLSUM .GE. GGG) THEN
02977                   IDT = IDTJ
02978                   JCOUT = JCNT
02979                   QFLOOUT = MIN (ABS (TUBAR(13,IDT)), FLOSUM) /FLOSUM
02980                   FLSUM = FLSUM - DFLOW
02981                   GO TO 1336
02982                 ENDIF
02983    1335       CONTINUE
02984               WRITE(17,*) 'CANT FIND NEW TUBE'
02985               WRITE(17,*) XXX, FLSUM
02986               IDON = 1
02987               GO TO 1321
02988    1336       CONTINUE
02989   C
02990   C---  COMPUTE NEW GGG AND ZZZ POSITION FOR NO MIXING  ---
02991   C
02992               IF (IMIX .NE. 1) THEN
02993                 IF (NFIN.EQ.1 .AND. NFOUT.EQ.1) THEN
02994                   GGG = GGG
02995                 ELSEIF (NFIN.EQ.1 .AND. NFOUT.EQ.2) THEN
02996                   GGG = (GGG - FLSUM) /QFLOOUT
02997                 ELSEIF (NFIN.EQ.2 .AND. NFOUT.EQ.1) THEN
02998                   IF (JCOUT .EQ. 1) THEN
02999                     GGG = QFLOIN *GGG
03000                   ELSEIF (JCOUT .EQ. 2) THEN
03001                     QFLOIN2 = 1. - QFLOIN
03002                     GGG = QFLOIN *GGG + QFLOIN2
03003                   ELSE
03004                     PRINT*,'JCOUT IS NOT 1 OR 2',JCOUT
03005                     WRITE(17,*) 'JCOUT IS NOT 1 OR 2',JCOUT
03006                   ENDIF
03007                 ELSE
03008                   PRINT*,'NUMBER OF TUBES IS WRONG'
03009                   WRITE(17,*) 'NUMBER OF TUBES IS WRONG'
03010                 ENDIF
03011               ENDIF
03012   C
```

```
03013                IF (GGG .GT. 1.0 .OR. GGG .LT. 0.) THEN
03014                  PRINT*,'GGG OUT OF RANGE',GGG
03015                  WRITE(17,*) 'GGG OUT OF RANGE',GGG,NFIN,NFOUT,QFLOIN,
03016         1                    QFLOOUT,FLSUM,JCOUT
03017                ENDIF
03018                GGG = MIN (0.999, MAX (0.001, GGG))
03019                ZZZ = 2. *GGG -1.
03020    C
03021     1363       CONTINUE

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03022                JBLOK(IDT) = 1
03023                JNOD = TUBNOD(1,IDT)
03024                IF (JNOD .EQ. INOD) JNOD = TUBNOD(2,IDT)
03025                ISN = 1
03026                IF (TUBNOD(1,IDT) .NE. INOD) ISN = - 1
03027                VEL = ISN *TUBAR(10,IDT)
03028                VEL = SIGN (MAX (ABS (VEL), 1.E-30), VEL)
03029    C
03030    C---  START MOVE PARTICLE  ---
03031    C
03032                ISTIK = 0
03033                IMOV = 0
03034                IEXIT = 0
03035                DYDS = (YNOD(JNOD)-YNOD(INOD)) /TUBAR(1,IDT)
03036                DXDS = (XNOD(JNOD)-XNOD(INOD)) /TUBAR(1,IDT)
03037                XB(1) = XNOD(INOD) + 1.000 *TUBAR(7,IDT)
03038                YB(1) = YNOD(INOD) + 1.000 *TUBAR(8,IDT)
03039                XB(2) = XB(1)
03040                YB(2) = YB(1)
03041    C
03042    C---  CHECK FOR TUBE BLOCKAGE  ---
03043    C
03044                IF (DPART .GT. TUBAR(2,IDT)) THEN
03045                  ISTIK = 1
03046                  IDON = 1
03047                  XB(2) = XNOD(INOD) + DXDS *TUBAR(1,IDT) /2.
03048                  YB(2) = YNOD(INOD) + DYDS *TUBAR(1,IDT) /2.
03049                ELSE
03050                  IARIV = 0
03051                  DELTIMF = TUBAR(1,IDT) /ABS (VEL) /100.
03052                  DIFFL = TUBAR(14,IDT)
03053                  DELTIMD = (DIFFL /(20.*PI/3.))**2 /DCOF /2.
03054                  DELTIM = MIN (DELTIMF, DELTIMD)
03055                  IF (PECL .GT. 9.E9) THEN
03056                    DELTIM = TUBAR(1,IDT) /ABS (VEL) /0.9
03057                  ENDIF
03058    C
03059                  SSS = 0.
03060                  ZZZIN = ZZZ
03061    C
03062    C---  TAKE INTERMEDIATE STEPS ALONG TUBE LENGTH  ---
03063    C
03064                  TSUM = 0.
03065                  BSUM = 0.
03066                  DO 1340 KSTP = 1, 1000000
03067                    IF (IARIV .NE. 0) GO TO 1341
03068                    IF (IDON .EQ. 1) GO TO 1341
03069                    IF (DELTIM .GT. TREM) THEN
03070                      DELTIM = MAX (TREM, 1.E-30)
```

```
03071                     IDON = 1
03072                   ENDIF
03073    1343           CONTINUE
03074    C
03075    C---  COMPUTE LOCAL APERTURE  ---
03076    C
03077                   HHH = 0.
03078                   IF (KMETH .EQ. 2) THEN

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03079                     ID = TUBNOD(3,IDT)
03080                     HH1 = 0.
03081                     IF (ID .GE. 1) THEN
03082                       TRM = RADI(ID)**2 - (SSS-TUBAR(1,IDT)/2.)**2
03083                       TRM = MAX (TRM, 1.E-30)
03084                       HH1 = RADI(ID) + TUBAR(2,IDT)/2. - SQRT(TRM)
03085                     ENDIF
03086                     ID = TUBNOD(4,IDT)
03087                     HH2 = 0.
03088                     IF (ID .GE. 1) THEN
03089                       TRM = RADI(ID)**2 - (SSS-TUBAR(1,IDT)/2.)**2
03090                       TRM = MAX (TRM, 1.E-30)
03091                       HH2 = RADI(ID) + TUBAR(2,IDT)/2. - SQRT(TRM)
03092                     ENDIF
03093                     HHH = MAX (HH1+HH2, 1.E-30)
03094                   ENDIF
03095    C
03096    C---  TAKE ADVECTIVE STEP  ---
03097    C
03098                   IF (IPARA .EQ. 1) THEN
03099                     VLOC = 1.5 *VEL *(1. - ZZZ**2)
03100                   ELSE
03101                     VLOC = VEL
03102                   ENDIF
03103                   IF (KMETH .EQ. 2) VLOC = VLOC *TUBAR(14,IDT) /HHH
03104                   DELSADV = VLOC *DELTIM
03105                   DELS = DELSADV
03106                   IF (SSS+DELS .GT. TUBAR(1,IDT)) THEN
03107                     IARIV = 1
03108                     DELS = TUBAR(1,IDT) - SSS
03109                     DELTIM = ABS (DELS /VLOC)
03110                     IF (NODAR(8,JNOD) .EQ. -IDBOU) THEN
03111                       IEXIT = 1
03112                       IDON = 1
03113                     ENDIF
03114                   ENDIF
03115                   BSUM = BSUM + HHH *DELS
03116                   TSUM = TSUM + DELTIM
03117
03118    C
03119    C---  TAKE DIFFUSIVE STEP  ---
03120    C
03121                   IDIR = 1
03122                   IF (RAN(ISED) .LT. 0.5) IDIR = -1
03123                   DELSDIF = IDIR *SQRT (2. *DCOF *DELTIM)
03124                   DELZ = DELSDIF /(TUBAR(14,IDT) /2.)
03125                   IF (KMETH .EQ. 2) DELZ = DELZ *TUBAR(14,IDT) /HHH
03126                   IF (ZZZ+DELZ .GT. 1.0) THEN
03127                     DELZ =  2.*(1.-ZZZ) - DELZ
03128                   ELSEIF (ZZZ+DELZ .LT. -1.0) THEN
```

```
03129                     DELZ = -2.*(1.+ZZZ) - DELZ
03130                   ENDIF
03131                   IF (PECL .GT. 9.E9) THEN
03132                     DELZ = 0.
03133                   ENDIF
03134   C
03135   C--- UPDATE POSITION AND TIME  ---

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03136   C
03137                   SSS = SSS + DELS
03138                   ZZZ = ZZZ + DELZ
03139                   IF (IRANS .EQ. 1) ZZZ = (2. *RAN(ISED) - 1.)
03140                   TREM = TREM - DELTIM
03141   C
03142    1340         CONTINUE
03143                ENDIF
03144    1341        XB(2) = XB(1) + DXDS *SSS
03145                YB(2) = YB(1) + DYDS *SSS
03146                IF (KMETH .EQ. 2) THEN
03147                  DELZ = ZZZ *HHH /2.
03148                  XB(2) = XB(2) - DELZ *DYDS
03149                  YB(2) = YB(2) + DELZ *DXDS
03150                ENDIF
03151                TORT = TORT + SSS
03152                XYNPAR(1,J) = XB(2)
03153                XYNPAR(2,J) = YB(2)
03154                XYNPAR(3,J) = INOD
03155                IF (IARIV .EQ. 1) THEN
03156                  INOD = JNOD
03157                ELSEIF (IARIV .EQ. -1) THEN
03158                  INOD = INOD
03159                ENDIF
03160   C
03161                BSUM = BSUM /TUBAR(1,IDT)
03162                WRITE(17,900) TUBAR(2,IDT),TUBAR(14,IDT),BSUM,TSUM,
03163         1        TUBAR(1,IDT)/VEL
03164   C
03165   C---  RESET STREAMLINE TO ENTRANCE VALUE  ---
03166   C
03167                IF (IZZZ .EQ. 1) THEN
03168                  ZZZ = ZZZIN
03169                ENDIF
03170   C
03171   C---  PLOTT TRACER PARTICLE TRAJECTORY  ---
03172   C
03173                IF (IPLTTR .EQ. 1) THEN
03174                  CALL CURVE(XB,YB,2,0)
03175                ENDIF
03176   C
03177    1320      CONTINUE
03178   C
03179   C---  PLOTT FINAL PARTICLE POSITION  ---
03180   C
03181    1321      CONTINUE
03182              IF (IEXIT .EQ. 0) THEN
03183                CALL MARKER(15)
03184                CALL CURVE(XB(2),YB(2),1,-1)
03185              ELSEIF (IEXIT .EQ. 1) THEN
03186                ARRTIM(J) = DTIM - TREM
```

```
03187                ARTBAR = ARTBAR + ARRTIM(J)
03188                CALL MARKER(13)
03189                XB(2) = 0.99 *XMAX
03190                CALL CURVE(XB(2),YB(2),1,-1)
03191              ELSEIF (IEXIT .EQ.-1) THEN
03192                CALL MARKER(13)

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03193                XB(2) = 0.01 *XMAX
03194                CALL CURVE(XB(2),YB(2),1,-1)
03195              ENDIF
03196   C
03197              TORT = (TORT /MAX (1.E-10, XB(2)))**2
03198              TORSUM = TORSUM + TORT
03199   C
03200   C---  STORE PATICLE POSITION IN FREQUNCY DISTRIBUTION  ---
03201   C     AND SUM AVERAGE POSITION
03202   C
03203              KPSUM = KPSUM + 1
03204              IFR = NINT (XB(2) /XMAX *99) + 1
03205              FREQ(IFR) = FREQ(IFR) + 1.
03206              XBAR = XBAR + XB(2)
03207              VTRACE(KPSUM) = XB(2) /DTIM
03208              VTBAR = VTBAR + VTRACE(KPSUM)
03209   C
03210    1310    CONTINUE
03211            CALL RESET('DASH')
03212            CALL RESET('THKCRV')
03213            ARTBAR = MAX (1.E-10, ARTBAR /KPAR)
03214            XBAR = XBAR /KPAR
03215            VTBAR = VTBAR /KPAR
03216            TORT =. TORSUM /KPAR
03217   C
03218   C---  COMPUTE STANDARD DEVIATIONS ---
03219   C
03220            SDEV = 0.
03221            STIM = 0.
03222            SIGV = 0.
03223            SDTR = 0.
03224            DO 1348 IPAR = 1, KPAR
03225              SDEV = SDEV + (XBAR-XYNPAR(1,IPAR))**2
03226              SDTR = SDTR + (XYNPAR(2,IPAR)-XYNPAR(4,IPAR))**2
03227              STIM = STIM + (ARTBAR - ARRTIM(IPAR))**2
03228              SIGV = SIGV + (VTRACE(IPAR) - VTBAR)**2
03229    1348    CONTINUE
03230            SDEV = SQRT (SDEV /KPAR)
03231            SDTR = SQRT (SDTR /KPAR)
03232            STIM = SQRT (STIM /KPAR)
03233            SIGV = SQRT (SIGV /KPAR)
03234   C
03235   C---  COMPUTE CUMULATIVE DISTRIBUTION  ---
03236   C
03237            DO 1391 IFR = 1, 100
03238              XB(IFR) = (IFR-0.5) /100 *XMAX
03239              YB(IFR) = 1.
03240              DO 1392 JFR = 1, IFR
03241                YB(IFR) = YB(IFR) - FREQ(JFR) /KPAR
03242    1392      CONTINUE
03243              IF (YB(IFR) .GE. 0.5) X50 = XB(IFR)
03244              YB(IFR) = YB(IFR) *YMAX
```

```
03245    1391   CONTINUE
03246           X50 = MAX (1.E-10, X50)
03247   C
03248           IF (IMICF .NE. 1) THEN
03249             CALL THKCRV(.050)

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03250             CALL CURVE(XB,YB,100,0)
03251           ENDIF
03252   C
03253   C---  COMPUTE APPARENT DIFFUSIVITY AND PLOTT CORRESPONDING ERROR FUNC  ---
03254   C
03255           VPAR = XBAR /DTIM
03256           PEVP = PECL *VPAR /VBAR
03257           PEBB = PEVP *BBAR /DIAMF
03258           DIFF = SDEV**2 /2. /XBAR
03259           DIF2 = SDEV**2 /2. /DTIM
03260           DIFT = SDTR**2 /2. /DTIM
03261           DIF3 = (UREF /PORO *STIM)**2 /2. /ARTBAR
03262           DIF4 = SIGV**2 *DTIM /2.
03263           DIFF0 = MAX (1.E-20, SDEVT/DTBAR*DIAMF)
03264           DCON = DIFF /DIFF0
03265           CON1 = PORO *DIF2 /DCOF /(2.*PECL)
03266           CONS = PORO *DIF2 /DCOF /(2.*PECS)
03267           DO 1367 IFR = 1, 101
03268             XB(IFR) = (IFR-1.) /100 *XMAX
03269             ETA = (XBAR-XB(IFR)) / 2. /SQRT(XBAR*DIFF)
03270             YB(IFR) = 0.5 *(1. + ERF(ETA)) *YMAX
03271    1367   CONTINUE
03272           IF (IMICF .NE. 1) THEN
03273             CALL DASH
03274             CALL CURVE(XB,YB,100,0)
03275             CALL RESET ('DASH')
03276           ENDIF
03277   C
03278   C---  PLOTT USED TUBES FOR MICRO-FINGERS  ---
03279   C
03280           IF (IMICF .EQ. 1) THEN
03281             DO 1703 IDT = 1, NTUB
03282               XB(1) = TUBAR(3,IDT)
03283               YB(1) = TUBAR(4,IDT)
03284               XB(2) = TUBAR(5,IDT)
03285               YB(2) = TUBAR(6,IDT)
03286               WID = MIN (TUBAR(2,IDT), 3.*TUBAR(1,IDT))
03287               WID = 0.98 *MAX (WID, 0.)
03288               WID = WID /XMAX *XAXIS
03289               WID = MAX (WID, .001)
03290               CALL THKCRV(WID)
03291               IF (JBLOK(IDT) .EQ. 1) CALL CURVE(XB,YB,2,0)
03292    1703     CONTINUE
03293           ENDIF
03294   C
03295           CALL RESET('THKCRV')
03296           CALL SCLPIC(1.0)
03297           XB(1) = 0.
03298           YB(1) = 1.
03299           CALL SCLPIC(0.0001)
03300           CALL CURVE(XB,YB,1,1)
03301           CALL ENDGR(0)
03302           PRINT980,'PECL',PECL
```

```
03303           PRINT980,'PEVP',PEVP
03304           PRINT980,'PEBB',PEBB
03305           PRINT980,'DIFL',DIF2/DCOF
03306           PRINT980,'DIFT',DIFT/DCOF

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03307           PRINT980,'TORT',TORT
03308           PRINT980,' '
03309           PRINT980,'X50 ',X50
03310           PRINT980,'VPAR',VPAR
03311           PRINT980,'XBAR',XBAR
03312           PRINT980,'DCON',DCON
03313           PRINT980,'CONS',CONS
03314           PRINT980,'CON1',CON1
03315           PRINT980,'SDEV',SDEV
03316           PRINT980,'DIFF',DIFF
03317           PRINT980,'DIF2',DIF2
03318           PRINT980,'DIF3',DIF3
03319           PRINT980,'DRAT',DIFF/DCOF
03320           PRINT980,'DRA4',DIF4/DCOF
03321           PRINT980,'SIGV',SIGV
03322           PRINT980,'SVRA',SIGV/VTBAR
03323           PRINT980,'     '
03324           CALL ENDPL(0)
03325         ENDIF
03326   C
03327    710  CONTINUE
03328    830  CONTINUE
03329   C
03330         PRINT*,'INPUT ICONT   1 = NEW PRESS
03331        1    2 = NEW TUBES  3 = RESTART'
03332         READ*,ICONT
03333         IF (ICONT.EQ.1) THEN
03334           GO TO 1620
03335         ELSEIF (ICONT.EQ.2) THEN
03336           GO TO 1610
03337         ELSEIF (ICONT.EQ.3) THEN
03338           GO TO 1600
03339         ENDIF
03340   C
03341    840  CALL DONEPL
03342   C
03343    988  FORMAT('1',A,2X,1PE11.3)
03344    980  FORMAT(1X,A,2X,1PE11.3)
03345    981  FORMAT(1X,A,2X,I11,1PE11.3)
03346    900  FORMAT(11(1PE12.4))
03347    990  FORMAT(12(1PE11.3))
03348    901  FORMAT(I10,10(1PE12.4))
03349    902  FORMAT(2(I10),8(1PE12.4))
03350    922  FORMAT(2(I10),10(1PE11.3))
03351    912  FORMAT(2(I5),8(1PE12.4))
03352    903  FORMAT(3(I10),8(1PE12.4))
03353    913  FORMAT(3(I6),8(1PE12.4))
03354    904  FORMAT(4(I10),8(1PE12.4))
03355    905  FORMAT(5(I10),8(1PE12.4))
03356   1900  FORMAT(10(1PE12.4))
03357   1901  FORMAT(I4,10(1PE12.4))
03358   1902  FORMAT(2(I4),8(1PE12.4))
03359   1912  FORMAT(2(I5),8(1PE12.4))
03360   1903  FORMAT(3(I4),8(1PE12.4))
```

```
03361   1904  FORMAT(4(I4),8(1PE12.4))
03362   1910  FORMAT(20(I4),8(1PE12.4))
03363         STOP


00001   C
00002   ************************************************************************
00003   C
00004         SUBROUTINE SPACEF (NBIN,NSEED,XS,YS,XMAX,YMAX,SDEVX,SDEVY)
00005         REAL XS(1),YS(1),FREQX(100),FREQY(100)
00006   C
00007         DO 761 J = 1, NBIN
00008           FREQX(J) = 0.
00009    761    FREQY(J) = 0.
00010         DO 762 ID = 1, NSEED
00011           IX = NINT (XS(ID) /XMAX *(NBIN-1)) + 1
00012           IY = NINT (YS(ID) /YMAX *(NBIN-1)) + 1
00013           FREQX(IX) = FREQX(IX) + 1.
00014    762    FREQY(IY) = FREQY(IY) + 1.
00015         SDEVX = 0.
00016         SDEVY = 0.
00017         BARN = (1.*NSEED) /NBIN
00018         DO 763 J = 1, NBIN
00019           SDEVX = SDEVX + (FREQX(J)-BARN)**2
00020    763    SDEVY = SDEVY + (FREQY(J)-BARN)**2
00021         SDEVX = SQRT(SDEVX /(NBIN-1.))
00022         SDEVY = SQRT(SDEVY /(NBIN-1.))
00023         RETURN
00024         END


00001   C
00002   ************************************************************************
00003   C
00004         SUBROUTINE NERNEB (NDARR, NBORS, NSEED, XS, YS, X0, Y0,
00005        1                   DNEIGH, INEIGH)
00006         REAL DNEIGH(NDARR,1), XS(1), YS(1), X0(1), Y0(1)
00007         INTEGER INEIGH(NDARR,1)
00008   C
00009   C---  NERNEB LOCATES NBORS NEAREST NEIGHBORS.  XS(I) AND YS(I) ARE SEED
00010   C     LOCATIONS, DNEIGH(I,J) IS THE DISTANCE TO NEIGHBOR I OF SEED J,
00011   C     AND INEIGH(I,J) IS THE SORTED SEED NUMBER OF THE ITH NEIGHBOR OF
00012   C     SEED J.  NERBER USES A BUBBLE SORT TO RANK NEIGHBORS IN INCREASING
00013   C     DISTANCE.
00014   C
00015         DDMX = 1.E20
00016         DO 1107 J = 1, NBORS
00017           DO 1107 ID = 1, NSEED
00018    1107     DNEIGH(J,ID) = DDMX
00019   C
00020         DO 1108 ID = 1, NSEED
00021           X0(ID) = XS(ID)
00022    1108   Y0(ID) = YS(ID)
00023   C
00024         DO 1101 ID = 1, NSEED
00025           DO 1102 IDP = 1, NSEED
00026             IF (IDP .EQ. ID) GO TO 1102
00027             DIS = SQRT((XS(ID)-XS(IDP))**2 + (YS(ID)-YS(IDP))**2)
00028             IF (DIS .LT. DNEIGH(NBORS,ID)) THEN
00029               DNEIGH(NBORS,ID) = DIS
00030               INEIGH(NBORS,ID) = IDP
```

```
00031              DO 1103 J = 1, NBORS-1
00032                K = NBORS - J
00033                IF (DNEIGH(K+1,ID) .LT. DNEIGH(K,ID)) THEN
00034                  DTMP = DNEIGH(K,ID)
00035                  ITMP = INEIGH(K,ID)
00036                  DNEIGH(K,ID) = DNEIGH(K+1,ID)
00037                  INEIGH(K,ID) = INEIGH(K+1,ID)
00038                  DNEIGH(K+1,ID) = DTMP
00039                  INEIGH(K+1,ID) = ITMP
00040                ELSE
00041                  GO TO 1102
00042                ENDIF
00043   1103       CONTINUE
00044            ENDIF
00045   1102   CONTINUE
00046   1101 CONTINUE
00047        RETURN
00048        END


00001   C
00002   ************************************************************************
00003   C
00004        SUBROUTINE ERRINV(X)
00005        EXTERNAL FUNC
00006        DATA ERR,ERA /1.E-4,1.E-4/
00007        COMMON /BLKQ/ RMU,SIG,Z
00008        XL=RMU-20.*SIG
00009        XR=RMU+20.*SIG
00010        X=RMU
00011        CALL FZERO(FUNC,XL,XR,X,ERR,ERA,IFLAG)
00012        X=XL
00013        RETURN
00014        END


00001   C
00002   C
00003        FUNCTION FUNC(X)
00004        COMMON /BLKQ/ RMU,SIG,Z
00005        ETA=(X-RMU)/SIG/SQRT(2.)
00006        FUNC=(1.+ERF(ETA))/2.-Z
00007        RETURN
00008        END


00001   C
00002   C************************************************************************
00003   C
00004        FUNCTION ERRETA (Y)
00005        EXTERNAL GUNC
00006        DATA ERR,ERA /1.E-4,1.E-4/
00007        COMMON /BLKZ/ VALU
00008        VALU = Y
00009        XL = -20
00010        XR =  20
00011        X = 0.
00012        CALL FZERO (GUNC, XL, XR, X, ERR, ERA, IFLAG)
00013        ERRETA = XL
00014        RETURN
00015        END
```

```
00001   C
00002         FUNCTION GUNC (X)
00003         COMMON /BLKZ/ VALU
00004         GUNC = ERF(X) - VALU
00005         RETURN
00006         END
```

```
00001   C
00002   C*************************************************************************
00003   C
00004         SUBROUTINE PLTBOX(XMAX,YMAX,NBOX)
00005         DIMENSION XX(20),YY(20)
00006         PI=4.*ATAN(1.)
00007         DDD=0.5*SQRT(1.+TAN(2.*PI/NBOX)**2)
00008         DO 814 J=1,NBOX+1
00009           THET=2.*PI*(J-1)/NBOX+2.*PI/NBOX/2.
00010           XX(J)=(0.5+DDD*COS(THET))*XMAX
00011           YY(J)=(0.5+DDD*SIN(THET))*YMAX
00012    814  CONTINUE
00013         CALL THKCRV(.030)
00014         CALL CURVE(XX,YY,NBOX+1,0)
00015         CALL THKCRV(.010)
00016         RETURN
00017         END
```

```
00001   C
00002   C*************************************************************************
00003   C
00004         SUBROUTINE PLTENDS(IDMX,NSID,IPRM,XSID,YSID,IPOP)
00005         DIMENSION NSID(1),IPRM(12,1),XSID(12,1),YSID(12,1),IPOP(12,1)
00006         DIMENSION XB(2),YB(2)
00007         CALL THKCRV(.010)
00008         DO 815 ID=1,IDMX
00009           DO 815 L=1,NSID(ID)
00010             IDP=IPRM(L,ID)
00011             IF (IDP.GT.ID) GO TO 815
00012             IF (IPOP(L,ID).EQ.1) THEN
00013               XB(1)=XSID(L,ID)
00014               YB(1)=YSID(L,ID)
00015               XB(2)=XSID(L+1,ID)
00016               YB(2)=YSID(L+1,ID)
00017               CALL CURVE(XB,YB,2,0)
00018             ENDIF
00019    815  CONTINUE
00020         RETURN
00021         END
```

```
00001   C
00002   C
00003         SUBROUTINE DELTAS (IFLAG, R1, R2, DELTA0, L, DELTAD, DELTAP,
00004        1                   DELTAV)
00005   C
00006   C   IFLAG = 1 => ANALYTICAL SOLUTION FOR R2 = R1 (ZEROTH-ORDER PERTURBATION
00007   C                SOLUTION)
00008   C   IFLAG = 2 => FIRST-ORDER PERTURBATION SOLUTION
00009   C   IFLAG = 3 => EXACT SOLUTION (VIA NUMERICAL INTEGRATION IF NECESSARY)
```

```
00010   C
00011         IMPLICIT DOUBLE PRECISION (A - H, O - Z)
00012         DOUBLE PRECISION K, I, L, INT3, INT1, LS4, KS, K1
00013         DIMENSION SUM(4), ZUM(4)
00014         DSTAR(TERM1, R3S, T, COST, SINT) = TERM1 - COST -
00015        1                                   SQRT(R3S - SINT*SINT)
00016         ARG = 0.5*L/R1
00017         RATIO2 = DELTA0/R1
00018         RATIO3 = R2/R1
00019         R1S = R1*R1
00020         LS4 = L*L/4.
00021         ROOT1 = SQRT(R1S - LS4)
00022         THETA = ASIN(ARG)
00023         IF (IFLAG .NE. 3) THEN
00024            K = RATIO2/2. + 1.
00025            K1 = K + 1.
00026            KS = K*K
00027            V1 = KS - 1.
00028            EPS = RATIO3 - 1.
00029            BASIC = ATAN(SQRT(K1/(K - 1.))*TAN(THETA/2.))/SQRT(V1)
00030            BASICK = BASIC*K
00031            G = -THETA + 2.*BASICK
00032            DELTAD = L/G
00033            DENOM = K - COS(THETA)
00034            V2 = SIN(THETA)/DENOM
00035            V3 = V2/DENOM
00036            F = (3.*BASICK + (1. + 0.5*KS)*V2)/V1 + 0.5*K*V3
00037            V1F = V1/F
00038            DELTAV = DELTA0 + R1*(2. - THETA/ARG) - ROOT1
00039            DELTAP = SQRT(4.*R1S*L*V1F/DELTAV)
00040            IF (IFLAG .EQ. 1) RETURN
00041            CD = (0.5*V2 - BASIC)/(K1*G)
00042            DELTAD = DELTAD*(1. + EPS*CD)
00043            H = (2.*(2.*KS + 1.)*BASIC + 3.*K*V2)/V1 + V3
00044            CE = (V3*V1F/DENOM + 2. - 1.5*H/F)/(6.*K1)
00045            DV1 = R1*(1. - THETA/ARG)
00046            CP = 0.5*(3.*CE - DV1/DELTAV)
00047            DELTAV = DELTAV + EPS*DV1
00048            DELTAP = DELTAP*(1. + EPS*CP)
00049            RETURN
00050         ELSE
00051            TERM1 = RATIO2 + 1. + RATIO3
00052            R3S = RATIO3*RATIO3
00053            R2S = R2*R2
00054            DT = THETA/20.
00055            T = 0.
00056            DELTA = DSTAR(TERM1, R3S, T, 1.D0, 0.D0)
00057            ZUM(2) = 0.5/DELTA

DELTAS

00058            ZUM(4) = 0.
00059            SUM(2) = ZUM(2)/(DELTA*DELTA)
00060            SUM(4) = 0.
00061            IFLIP = 2
00062            DO 11 J = 1, 20
00063               T = T + DT
00064               COST = COS(T)
00065               SINT = SIN(T)
00066               DELTA = DSTAR(TERM1, R3S, T, COST, SINT)
00067               GRAND2 = COST/DELTA
```

```
00068                GRAND1 = GRAND2/(DELTA*DELTA)
00069                IFLIP = 6 - IFLIP
00070                SUM(IFLIP) = SUM(IFLIP) + GRAND1
00071                ZUM(IFLIP) = ZUM(IFLIP) + GRAND2
00072          11    CONTINUE
00073                SUM(2) = SUM(2) - 0.5*GRAND1
00074                ZUM(2) = ZUM(2) - 0.5*GRAND2
00075                FACTOR = 1.5*L/DT
00076                DECUBE = FACTOR*R1S/(2.*SUM(2) + 4.*SUM(4))
00077                DELTAD = FACTOR/(2.*ZUM(2) + 4.*ZUM(4))
00078                ROOT2 = SQRT(R2S - LS4)
00079                DELTAV = DELTA0 + R1 + R2 - 0.5*(ROOT1 + ROOT2) -
00080              1          (R2S/L)*ASIN(0.5*L/R2) - (R1S/L)*THETA
00081                DELTAP = SQRT(DECUBE/DELTAV)
00082              END IF
00083              RETURN
00084              END


00001    C
00002    C
00003              FUNCTION BOXMUL (ISED, RMU, SDEV, R2)
00004              DATA TWOPI /6.2831853072/
00005              XXX1 = RAN (ISED)
00006              XXX2 = RAN (ISED)
00007              BOXMUL = SQRT(-2. *ALOG(XXX1)) *COS (TWOPI *XXX2)
00008              BOXMUL = SDEV *BOXMUL + RMU
00009              R2 = SQRT(-2. *ALOG(XXX1)) *SIN (TWOPI *XXX2)
00010              R2 = SDEV *R2 + RMU
00011              RETURN
00012              END
```

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