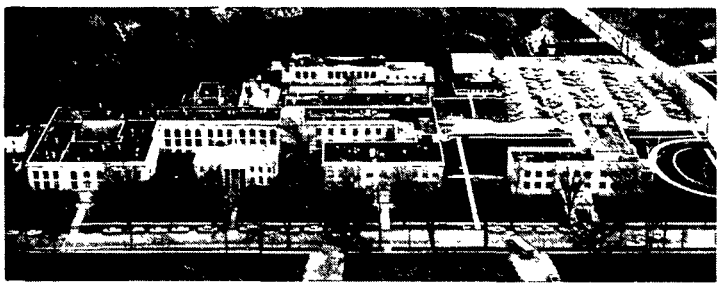

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RETENTION DYNAMICS FOR SMALL PARTICLES ON CYLINDRICAL FIBERS. I. A NEW MODEL FOR INVESTIGATING THE EFFECTS OF VARIOUS INTERACTIONS ON PARTICLE RETENTION

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Retention dynamics for small particles on cylindrical fibers. I. A new model for investigating the effects of various interactions on particle retention

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KEYWORDS:

ABSTRACT: Although particle retention is of importance to the paper industry, little is known concerning various factors that control it. A mathematical model has been developed to represent this complex process. The model simulates the passage of spherical particles around cylindrical fibers for flows within the creeping motion regime, and it determines whether or not individual particles will impact on the fiber surface. It is shown that the model leads to two second-order ordinary differential equations which, when integrated numerically, describe the path the particle traces as it moves around the fiber. This model enabled us to investigate hydrodynamic, molecular, and colloidal force effects independently and to outline their relative influence on retention. The effect on retention of system parameters such as porosity, fluid velocity, and particle size will be discussed.

Introduction

Particle collection within a fibrous porous medium is of significant importance to the paper industry. Proper amounts of filler material retained by the paper sheet will improve smoothness, brightness, opacity, ink receptivity, and porosity. Incorrect amounts will affect these adversely, decreasing the value of the product. Improved retention would also be of benefit environmentally — a decrease of waste load would aid mills to meet pollution control guidelines.

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Increased retention can be viewed as an economic and environmental concern of the paper industry. We need qualitative and quantitative information relating to the movement of a small, solid particle as it approaches a much larger fiber. Such an analysis should include the effect of various forces in removing a particle from the flow stream by attachment to the fiber. The goal of the present study was to obtain some of this information.

Previous investigations concerning particle retention have defined several mechanisms generally thought to influence particle motion (1-3). These include inertial impaction, flow line interception, diffusion, sieving, settling and thermal diffusion. Of these, the last three are generally considered negligible in a retention system such as the one under investigation. In addition to these mechanisms, retention systems are characterized by several force interactions which influence particle movement and collection. Van der Waals attractive force and the double-layer force are known to influence a particle-fiber interaction. These forces can cause retention directly or cause a particle to move into a position where one of the physical mechanisms would dominate. Such attractive and repulsive forces exist between any two particles of matter, whatever their size or chemical composition.

Retention has been shown to depend on a balance between attractive and repulsive forces. The present study was undertaken in an attempt to understand retention and to identify conditions which would improve its efficiency. Specifically, the investigation concerned the relative importance of hydrodynamic, molecular, and colloidal forces existing within a simplified retention system. Individual force effects were studied and correlated with their influence on retention efficiency.

The method used for attaining this objective involved the construction of a mathematical model simulating retention in a particle-fiber system. We used an idealized system as a first step toward the objective of simulating an actual industrial process. The model simulates the motion of small spherical particles around fibers characterized by circular cross sections and smooth surfaces. By monitoring the movement of the particle as it is affected by various forces, we could calculate a collection efficiency and compare it to several system parameters.

This article describes the mathematical model and some of the results obtained. A subsequent article will compare model predictions with an experimental program.

Model development

Recent studies provide a solid base for this approach to the problem. Modeling work has been completed in the areas of aerosol (1) and water filtration (4,5). Although most work has been concerned with spherical collectors (6,7), some has been done for cylindrical collectors (8). All of these have attempted to show how various force factors affect collection rates.

The present model simulates a system in which a dilute suspension of small, spherical particles flows through a transverse parallel array of cylindrical fibers. Three force effects were considered: the hydrodynamic drag, attractive or repulsive forces arising from surface charges, and molecular attractive forces. Diffusion was also examined as a possible contribution to particle transport. The basis of the model is a set of particle trajectory equations which describe the motion of a particle as it flows around a fiber or collides with it. Solution of these equations leads to the calculation of a collection efficiency, the value used to correlate all of the results.

Equations of fluid flow

The theoretical basis for the flow equations is the expressions representing the conservation of mass and momentum. Incompressible flow has been assumed, so that the equation of continuity:

$$\partial\rho/\partial t = -\nabla\cdot(\rho\vec{v}), \tag{1}$$

becomes:

$$\nabla\cdot\vec{v} = 0 \tag{2}$$

Further, by assuming creeping motion in a Newtonian fluid, the equation of motion:

$$\rho\, D\vec{v}/Dt = -\nabla\vec{p} - [\nabla\cdot\tau] + \rho\vec{g}\ , \tag{3}$$

takes the form:

$$\mu(\nabla^2\vec{v}) = \nabla p \tag{4}$$

By assuming a two dimensional system in cylindrical coordinates, Equations (2) and (4) can be expressed as the following series of equations; these represent fluid flow in the system to be investigated:

$$\partial v_r/\partial r + v_r/r + (1/r)\ \partial v_\theta/\partial\theta = 0 \tag{5}$$

$$\partial p/\partial r = \mu[\nabla^2 v_r - v_r/r^2 - (2/r^2)\partial v_\theta/\partial\theta] \tag{6}$$

$$(1/r)\partial p/\partial\theta = \mu[\nabla^2 v_\theta - v_\theta/r^2 + (2/r^2)\partial v_r/\partial\theta] \tag{7}$$

Description of the unit cell

The mathematical model described here has been designed to represent the flow around a transverse parallel array of circular fibers, with flow perpendicular to the fiber axis. Theoretically, it is possible to remove a single fiber from the array,

describing it as an average of all other fibers in that assemblage. In this way, a physical system is replaced with an equivalent arrangement based on a single collector. Known as the unit cell technique, this type of simplification has been used extensively by Happel (9), Kuwabara (10), and other investigators.

The unit cell employed in the present study is shown schematically in fig. 1. It consists of two concentric cylinders; the inner one, of radius A, represents the solid fiber, and the outer one, with radius B, has been called the fluid envelope and is characterized by a free surface. The porosity of the system is related to the ratio of the fluid area to the total area of the cell and is equal to that of the assemblage. It has been assumed that the usual no-slip condition exists at the fiber surface, and at the fluid envelope the shear stress is zero. At any point within the fluid annulus of the cell, the velocity can be resolved into its r- and θ-components. At time t, an element of the fluid may be situated in the unit cell. At an increment of time later, dt, the same element will be at a new position, traveling a distance $\vec{dr}$ through an angle dθ.

Fluid velocity equations

In terms of a stream function, ψ, the fluid velocity components can be defined as:

$$v_r = \left(1/r\right) \partial\psi/\partial\theta \qquad\qquad v_\theta = -\partial\psi/\partial r \qquad (8)$$

The equations defining creeping motion assume the form of a fourth-order, scalar equation:

$$\nabla^4\psi = \nabla^2(\nabla^2\psi) = 0 \qquad (9)$$

Lines of constant ψ describe the fluid streamlines surrounding the fiber. The following is a solution of Equation (9):

$$\psi = \sin\theta\,[Cr^3 + Dr + E/r + Fr\ \ln r], \tag{10}$$

where C, D, E, and F represent integration constants. The values of the constants were obtained by applying appropriate boundary conditions to the stream function. Two of these result from the no-slip conditions assumed to exist at the fiber surface:

$$\text{at } r = A \qquad \begin{cases} v_r = 0 & (11) \\ v_\theta = 0 & (12) \end{cases}$$

Two more were defined by noting that there is a finite velocity at the fluid envelope, while at the same point, the shear stress is zero:

$$\text{at } r = B \qquad \begin{cases} v_r = -U\cos\theta & (13) \\ \tau_{r\theta} = \mu[(1/r)\ \partial v_r/\partial\theta + \partial v_\theta/\partial r - v_\theta/r] = 0 & (14) \end{cases}$$

These boundary conditions permitted the derivation of the specific stream function applicable to flow through the unit cell:

$$\psi = \frac{U\sin\theta}{f(\varepsilon)}\left\{(1-\varepsilon)^2\frac{r^3}{A^2} - \frac{A^2}{r} - 2[1 + (1-\varepsilon)^2]r\ \ln\frac{r}{A}(1-\varepsilon)^{\frac{1}{2}} - r\,f(\varepsilon)\right\} \tag{15}$$

where

$$\varepsilon = \text{porosity} = (1 - A^2/B^2) \tag{16}$$

$$f(\varepsilon) = (1-\varepsilon)^2 - 1 - 2[1 + (1-\varepsilon)^2]\ \ln(1-\varepsilon)^{-\frac{1}{2}} \tag{17}$$

The fluid velocity components can be determined by taking the derivative of Equation (15) by using Equation (8):

$$v_r = \frac{U\cos\theta}{f(\varepsilon)}\left\{(1-\varepsilon)^2\frac{r^2}{A^2} - \frac{A^2}{r^2} - 2[1 + (1-\varepsilon)^2]\ \ln\frac{r}{A}(1-\varepsilon)^{\frac{1}{2}} - f(\varepsilon)\right\} \tag{18}$$

$$v_\theta = \frac{-U\sin\theta}{f(\varepsilon)}\left\{3(1-\varepsilon)^2\frac{r^2}{A^2} + \frac{A^2}{r^2} - 2[1 + (1-\varepsilon)^2][\ln\frac{r}{A}(1-\varepsilon)^{\frac{1}{2}} + 1] - f(\varepsilon)\right\} \tag{19}$$

Equations of particle motion

The next consideration was to examine the effect of locating a small spherical particle in the flow stream circling the fiber. A particle moving through a stationary liquid experiences a resistance to flow described by Stokes Law. If the fluid is in motion at a specified velocity, the particle will flow with a different velocity due to inertial effects. The drag force can then be written as:

$$\vec{F} = - 3\pi\mu d \ (\vec{v} - d\vec{r}/dt), \tag{20}$$

where $\vec{v}$ is the fluid velocity and $d\vec{r}/dt$ refers to the particle velocity. A second expression related to particle motion is Newton's second law, stating that force equals the rate of change of momentum:

$$\vec{P} = (d/dt) \ (m \ d\vec{r}/dt), \tag{21}$$

where m is particle mass.

Assuming that inertia is the only effect acting on the particle, the forces in Equations (20) and (21) can be set equal. The result is two nonlinear differential equations. These equations describe the movement of a particle through the unit cell in terms of radial and angular components:

$$d^2r/dt^2 = K_1(v_r - dr/dt) + r \ (d\theta/dt)^2 \tag{22}$$

$$d^2\theta/dt^2 = K_1[(v_\theta/r) - d\theta/dt] - (2/r)(dr/dt) \ d\theta/dt \tag{23}$$

$$K_1 = 18 \ \mu \ A/(d^2 \ \rho_p \ U) \tag{24}$$

Integration of these dimensionless equations provides the trajectory of a particle as it travels around the fiber.

As mentioned previously, both attractive and repulsive forces exist in a particle-fiber system such as the one being modeled. Attraction was considered the result of Van der Waals retarded force, while repulsion would be caused by the overlapping of similar double layers surrounding both particle and fiber. A suitable equation for Van der Waals attraction was modified from existing relationships (7,11) and applied to the trajectory equation in the following form:

$$F_{VdW} = -\frac{2H}{3\ m\ U^2}\ \frac{a_p^{\ 3}}{\delta^2(2a_p + \delta)^2}\ \alpha(a_p,\delta), \tag{25}$$

where H is the Hamaker constant and α is the retardation factor. This factor has been shown to be a complicated function of particle size and separation distance (12). The magnitude of this force drops off rapidly with separation distance; at a separation of less than a few hundred Angstroms, retardation is minimal. The effect of double layer repulsion was included in the following form (6):

$$F_{DL} = \frac{\varepsilon_d\ \kappa\ a_p\ A^2}{(300)^2\ m\ U^2}\left\{\zeta_1\zeta_2\ \frac{e^{-A\kappa\delta}}{1 + e^{-A\kappa\delta}} - \tfrac{1}{2}(\zeta_1 - \zeta_2)^2\ \frac{e^{-2A\kappa\delta}}{1 - e^{-2A\kappa\delta}}\right\}, \tag{26}$$

where ζ_1 and ζ_2 represent zeta-potential values for the particle and fiber, respectively. For two interacting bodies possessing like surface charges, this force is repulsive; if they are opposite, then there is an attraction.

Both of the forces mentioned are body-centered forces. For this reason, their effect is exerted in the radial direction only, making it necessary to include these force effects in the radial component equation of particle motion. Thus, the equations representing particle motion as affected by all forces mentioned would be:

$$d^2r/dt^2 = K_1(v_r - dr/dt) + r\,(d\theta/dt)^2 - F_{VdW}\,\alpha + F_{DL} \qquad (27)$$

$$d^2\theta/dt^2 = K_1[(v_\theta/r) - d\theta/dt] - (2/r)(dr/dt)\,d\theta/dt \qquad (28)$$

Solution of the trajectory equations

Numerical integration of Equations (27) and (28) was done by the fourth-order Runge-Kutta method, with the aid of a digital computer. The advantages of the procedure include accuracy, simplified starting, and programming convenience. A disadvantage of this method is the necessity of a small time step, resulting in a large number of iterations per trajectory. The initial input variables for the programming scheme consist of the particle's position and velocity components. Each iteration produces new values for these terms. The new values serve as input for the next step, and the procedure is repeated. The resulting series of particle position values trace the particle trajectory, indicating whether or not the particle impacted the fiber. By varying the initial position of the particle, collection efficiencies could be obtained for the system conditions assumed.

Predicted collection efficiency

The mathematical model has been developed to permit the calculation of a collection efficiency, which reflects the amount of retention occurring within the simulated system. The efficiency, η_p, is defined as a ratio of the flow area from which all particles are removed through impaction on the fiber to the projected area of the fiber. Fig. 2 represents the procedure used in calculating this value. The heavy line in the diagram is the limiting trajectory. A particle following this path will impact at the downstream axis of the unit cell. The initial position of the limiting trajectory is located on the fluid envelope, offset from the fiber axis by the angle θ. Any particle entering the cell at an angle less than θ will impact, while those entering

at larger angles will remain suspended in the flow. Thus the flow area from which particles are removed is denoted by N, and the efficiency is defined by:

$$\eta_p = N/A \tag{29}$$

Results and discussion

Effect of various forces on predicted retention values

The computer program written to integrate Equations (27) and (28) provides for each force thought to be active in retention. The particle trajectories, which represent the movement of the particle's center, can be plotted on a modified diagram of the unit cell. Plotting several trajectories on the same diagram, each calculated with different force effects, shows the influence of each force on particle motion.

Information of this type was first obtained (12) to examine the effect of inertia on particle motion. Integration of Equations (22) and (23) provides trajectories which incorporate only this effect. It was found that these trajectories were identical with fluid streamlines surrounding the fiber. This indicated that density differences between fluid and particle were not large enough for the particle to deviate from the flow stream. Therefore, it was concluded that inertia exerts no significant influence on retention in the flow regime studied.

Inclusion of the Van der Waals force produced variations in particle trajectories. Fig. 3 represents the results obtained when the model was used to calculate trajectories for a system of porosity 0.75, particle diameter 0.5 μm, approach velocity 1.00 cm/sec, and fiber diameter 20 μm. Van der Waals force was included in the calculation of Curve A, while Curve B reflects only the effect of inertia. This indicates that a particle influenced by these attractive forces will deviate from the fluid flow and impact on the fiber. Thus the model

predicts a significant collection efficiency, indicating that Van der Waals force would be an important factor in retention.

The next step in the investigation was the incorporation of double-layer repulsion into the motion equations. This resulted in Equation (27). Both attractive and repulsive force terms in this equation are functions of separation distance. A separation exists at which these forces will balance. This means that certain particles will approach a constant separation distance from the fiber. Utilizing values of zeta-potential for the particle (ζ_1 = -25 mV, based on titanium dioxide) and fiber (ζ_2 = -15 mV, based on nylon) and a value of the Debye-Hückel reciprocal length, $\kappa = 4.5 \times 10^6$ cm^{-1}, based on a particle suspension of acidic pH and 0.02 molar in monovalent salt, we calculated this distance to be 6×10^{-6} cm, which is roughly one-tenth of the particle diameter. The salt is used to compress the double layer and reduce its strength. The simulation based on the use of a divalent salt in the particle suspension predicts a constant separation at 3.0×10^{-6} cm.

These values indicate that, for an ideal system, the model predicts no particle impaction based on the equations employed here. However, it was felt that, in a real system, variations in particle size and shape, fiber roughness, or flow perturbations would influence particle motion over greater distances than those mentioned. These irregularities would reduce the separation to the point where the molecular forces would dominate and impaction would occur. The model predicted that, until the force balance occurred, trajectories calculated with and without the repulsive force were identical. The conclusion was that for a simulated system in which the double layers have been assumed collapsed, the repulsive interaction exerts little effect on retention.

A decreased ionic concentration in the particle suspension provides for an increase in double-layer thickness. If no electrolytes are added to the

suspension, the force balance occurs at a separation distance equivalent to about ten particle diameters. It is unlikely that any particle could penetrate this barrier to impact on the fiber, and the result would be negligible retention. Experimental studies (3,13) have confirmed this in a variety of systems when electrolytes are omitted from particle or fiber suspensions.

Diffusion has traditionally been considered a major influence in particle retention systems. The distance a particle travels within a specified time due to this random motion can be calculated by means of Einstein's diffusion coefficient and random walk theory (1,3). An estimate of the effect of diffusion under assumed conditions was derived from repeated trials in which a displacement in a random direction was included at each integration step. For convenience the magnitude of each such displacement was taken to be the expectation value corresponding to the given time step. It appears that this motion exerts no major influence on a particle trajectory. There was a slight tendency for the particle to drift away from the fiber when this motion was included, but this effect was not large enough to alter collection efficiency values significantly. Thus it was concluded that diffusion was not an important complication in this system.

Effect of system variables on collection efficiency

Table 1 is a summary of calculated collection efficiencies. These were obtained by integrating Equations (27) and (28) and assuming that the double layers around particles and fibers were collapsed. The system variables investigated have included porosity, approach velocity, and particle size. The effect of varying suspension ionic conditions was discussed previously.

The values in the table readily show that predicted retention values decrease as porosity increases. This can be explained by the fact that as porosity decreases, the flow area is reduced and more particles travel closer to the fiber

surface. Therefore, a larger number of particles experience the effect of Van der Waals force sooner and have an increased opportunity to collide with the fiber. The result is an increase in collection efficiency.

A particle enters the unit cell with a velocity equal to the bulk suspension, at a magnitude within the creeping motion regime. Once in the cell, the particle is exposed to various forces, and its velocity changes with respect to the fluid. Predicted collection efficiency decreases with increasing velocity. Fig. 4 shows how such a change will affect particle trajectories. Curves A, B, C, and D represent trajectories calculated with approach velocities of 0.78, 1.00, 1.17, and 1.50 cm/sec, respectively; all paths originate at an angle of 0.0050 radian. Curves E, F, G, and H represent the same velocities for trajectories originating at $\theta = 0.0070$ radian. As shown, the velocity change causes a marked difference in the trajectory, reflecting a change in efficiency. This is explained by the time it takes the particle to travel through the unit cell and be influenced by the attractive force. The greater the velocity, the shorter the exposure, resulting in a decrease in the number of particles captured.

Particle size is one of the most important factors in retention. The model predicts that efficiency is greater for larger particles, as shown in fig. 5. Trajectories A, B, and C were calculated for diameters of 1.0, 0.5, and 0.3 μm, respectively, all originating at an initial angle of 0.0050 radian. The figure shows that the number of particles collected decreases as their size decreases. This trend appears to be a direct result of the magnitude of the Van der Waals force. Equation (24) indicates that this force is directly proportional to the cube of the particle radius; thus, it would be much stronger for a larger particle. A stronger force would indicate increased collection.

Summary

This study has been concerned with the consequences of a mathematical model developed to simulate the retention of small, spherical particles on fibers of circular cross section. Various forces existing in such a system were considered independently to clarify their influence on particle collection. In addition, several system variables were varied to show how particle motion is affected by changes in them.

It has been shown that Van der Waals attractive force must be included in the model, which would otherwise predict no significant retention. Inertial impaction was found negligible in this system. A double-layer force would exist and has been assumed repulsive, in which case it would, of itself, produce no retention. Lastly, diffusion appears to exert only a small effect on collection efficiency values.

The model predicts that collection efficiency decreases with increasing porosity, increasing suspension approach velocity, and decreasing particle size. The ionic conditions of the particle suspension can be altered to increase the double-layer force and inhibit retention.

This study of a theory of retention was accompanied by an experimental program, developed to obtain comparison data. A description of this program and its role in the evaluation of the model appears in a subsequent paper.

List of symbols

A = fiber radius

a_p = particle radius

B = fluid envelope radius

C,D,E,F = integration constants

d = particle diameter

$\vec{dr}$ = small change in distance and direction of particle motion

F_{DL} = double-layer force

F_{VdW} = Van der Waals force

$\vec{F}$ = drag force vector

$\vec{g}$ = acceleration due to gravity

H = Hamaker constant

K_1 = coefficient in particle motion equations

m = particle mass

N = value used in the calculation of predicted collection efficiency

$\vec{P}$ = force vector, rate of change of momentum

p = pressure

r = radial position component

t = time

U = fluid approach velocity

$\vec{v}$ = local mass average fluid velocity

v_r = radial component of fluid velocity

v_θ = angular component of fluid velocity

α = retardation correction factor

δ = separation distance between particle and fiber

ε = porosity

ε_d = dielectric constant of water

ζ_1, ζ_2 = zeta-potentials for particle and fiber

η_p = predicted collection efficiency

θ = angular position component

κ = Debye-Hückel reciprocal length

μ = fluid viscosity

ρ = fluid density

ρ_p = particle density

τ = fluid stress

$\tau_{r,\theta}$ = shear stress at the fluid envelope

ψ = stream function

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Table 1. Predicted collection efficiencies

Porosity	Velocity (cm/sec)	Particle size		
		d = 1.0 μm	d = 0.5 μm	d = 0.3 μm
0.75	0.78	0.0286	0.0159	
	1.00	0.0270	0.0149	0.0103
	1.17	0.0262	0.0143	
	1.50	0.0252	0.013	
0.80	0.78	0.0231	0.0131	
	1.00	0.0220	0.0122	
	1.17	0.0215	0.0118	
	1.50	0.0202	0.010	
0.85	0.78	0.0187	0.012	
	1.00	0.0177	0.0100	0.0068
	1.17	0.0172	0.0095	
	1.50	0.0162	0.0089	0.0064

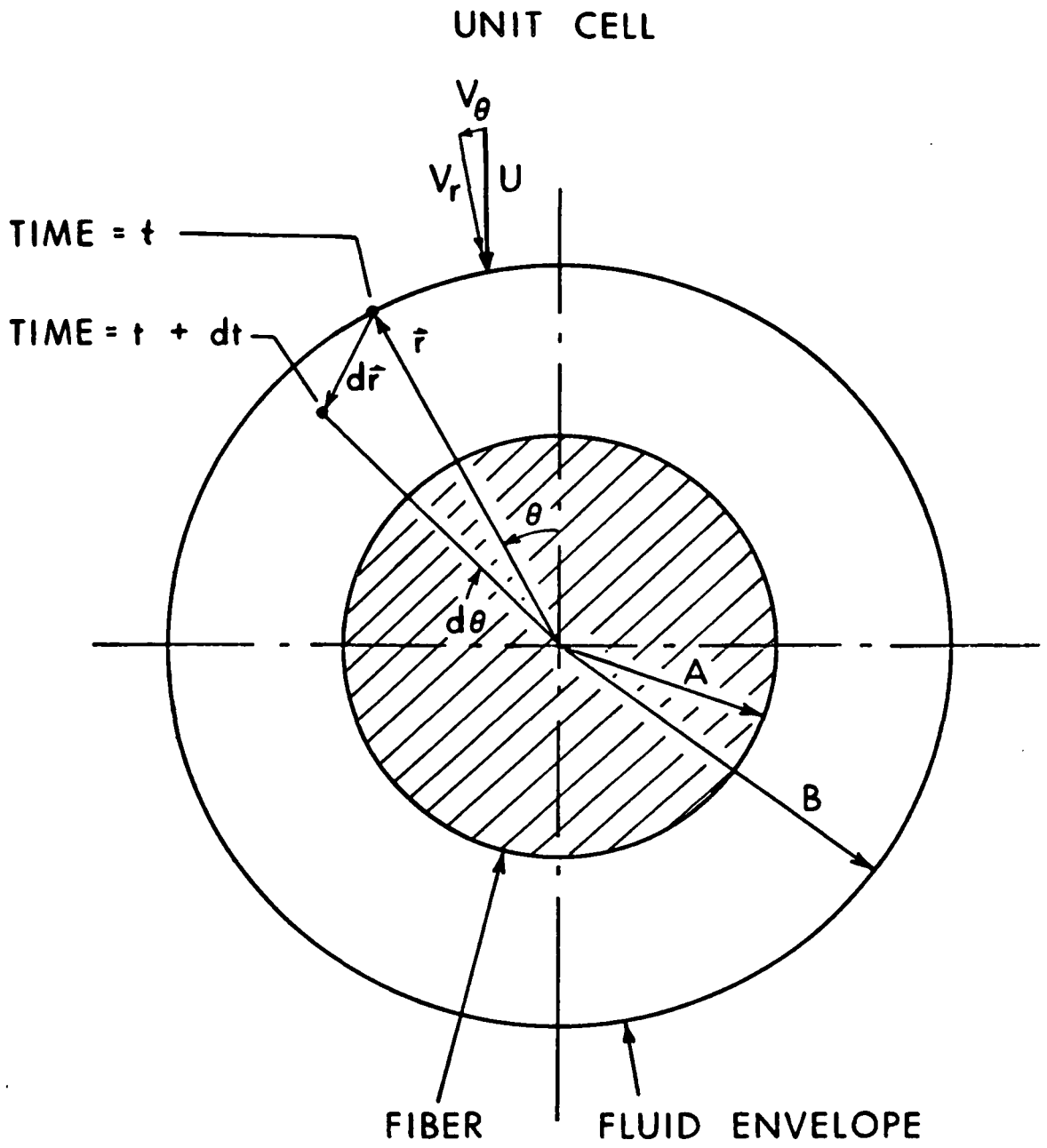

Fig. 1. The unit cell

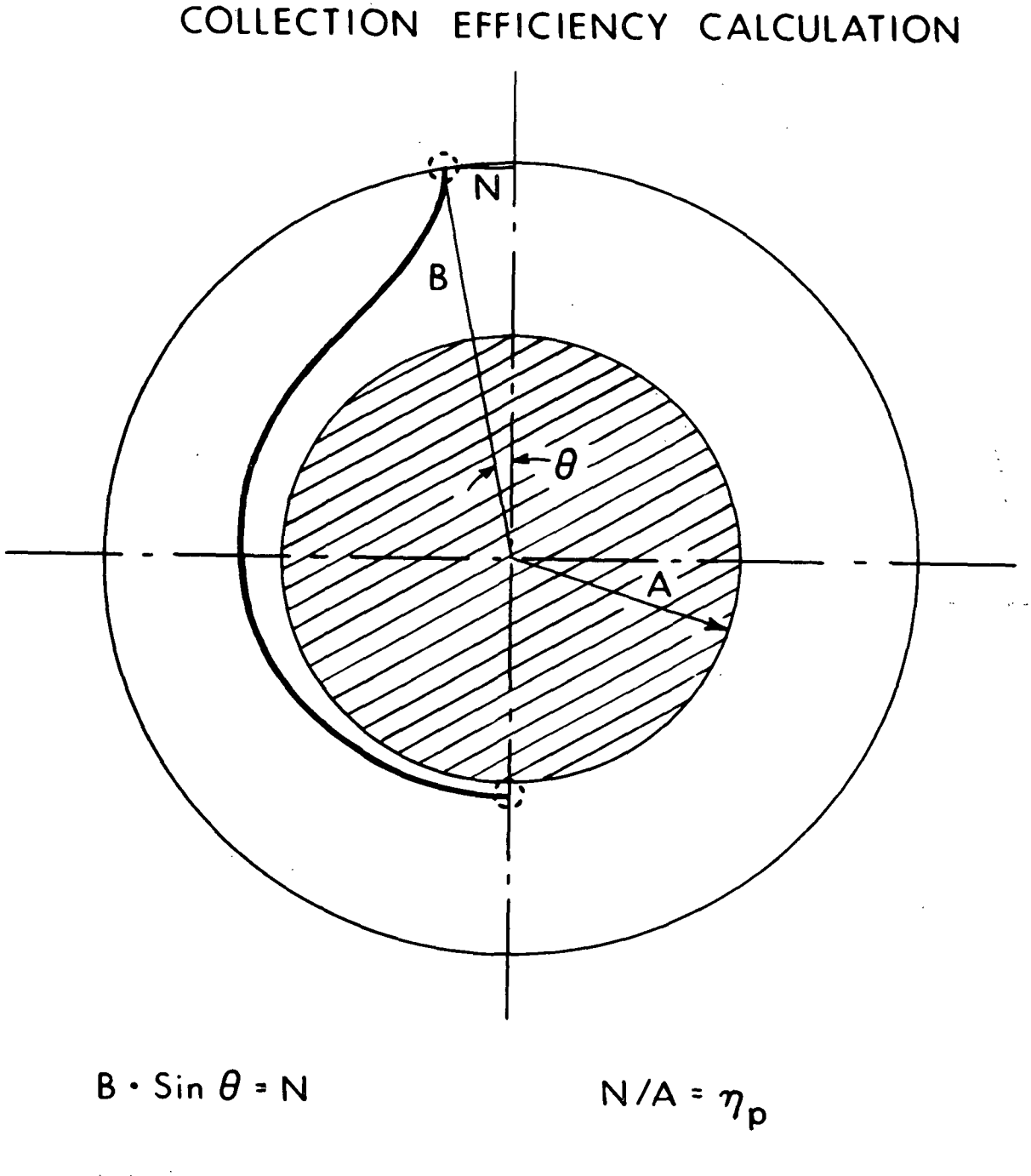

Fig. 2. A definition of collection efficiency

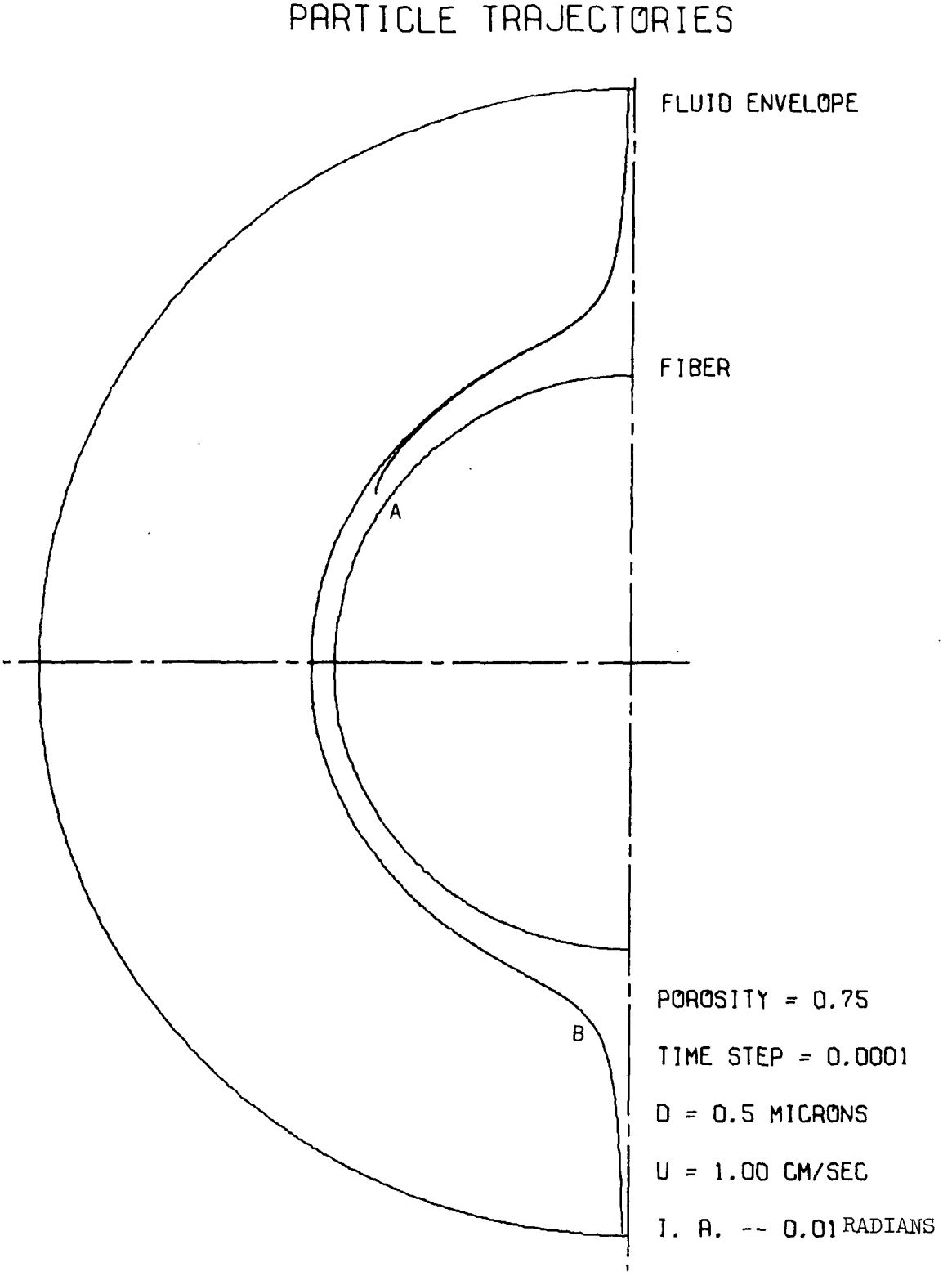

Fig. 3. The effect of including Van der Waals force in the calculation of particle trajectories (I.A. = initial angle of entry)

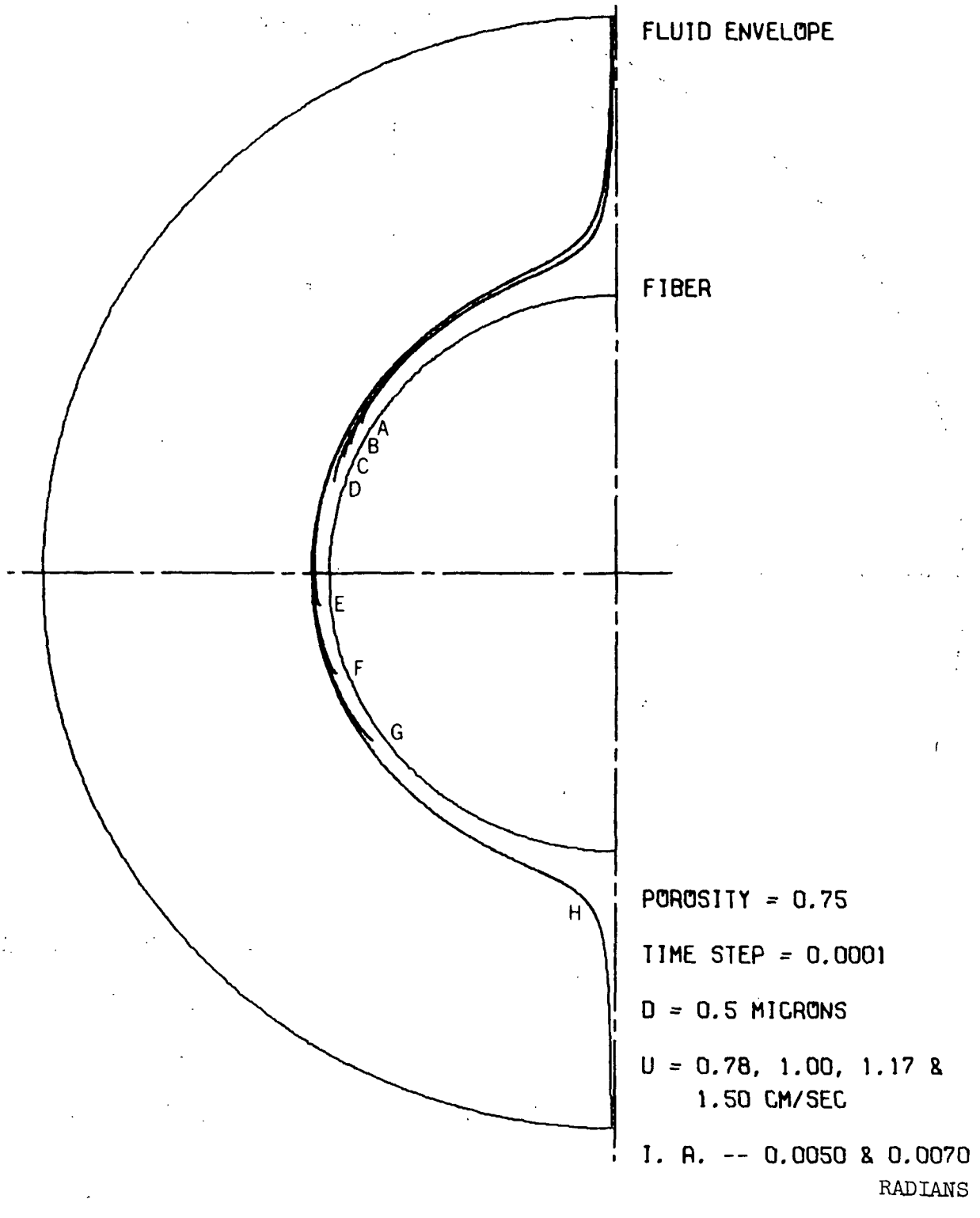

Fig. 4. The effect of varying approach velocity on particle trajectories

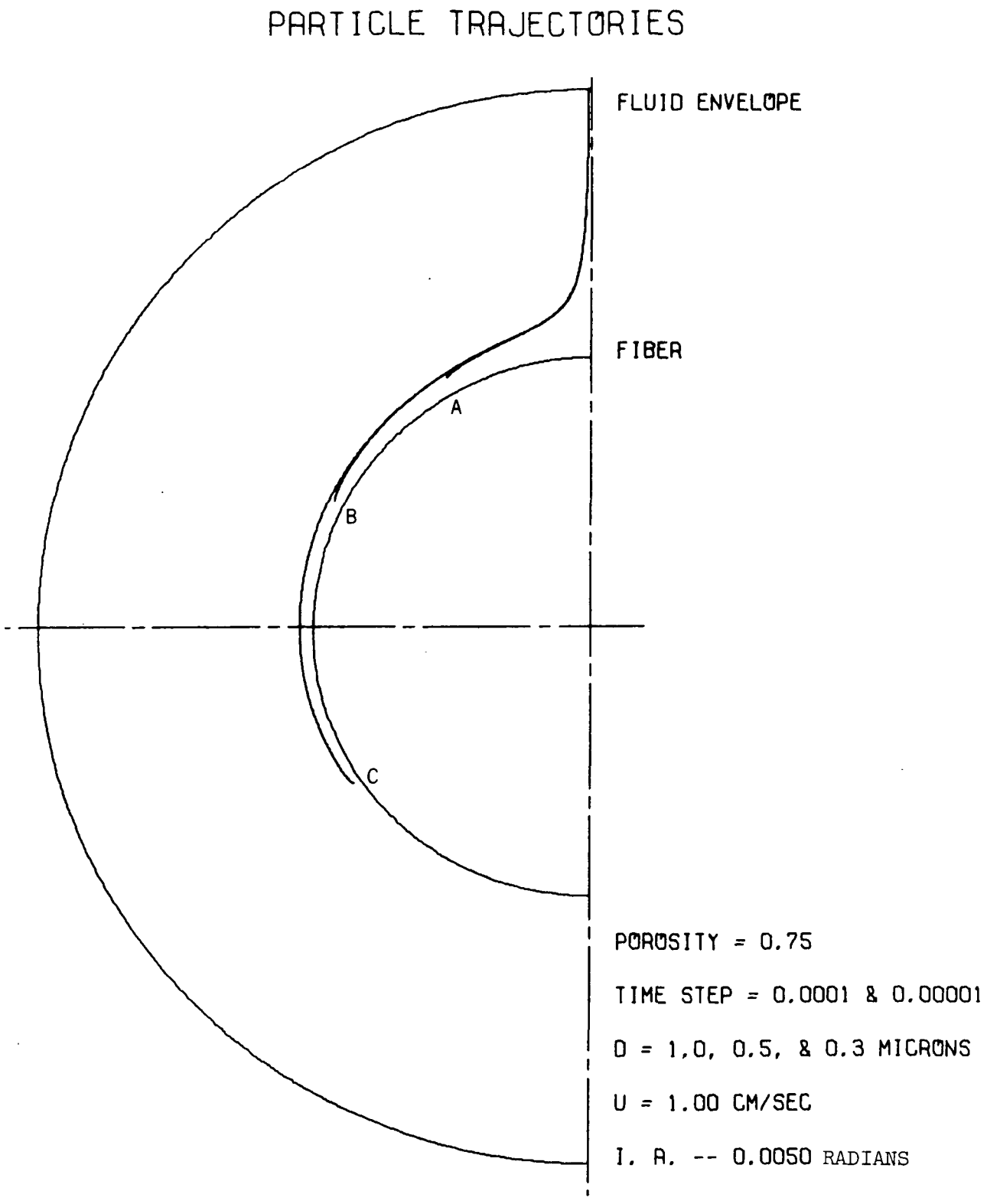

Fig. 5. The effect of changing particle size