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Hierarchial Analysis of Filtration

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For Subcontract B244781
Ending September 1993

July 1993

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Work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

Hierarchical Analysis of Filtration

by

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A progress report submitted to

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July 1993

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Abstract

The original proposal for this work suggested two lines of analysis that could be used to develop an hierarchical analysis of filtration. The first of these was *semi-empirical* and required the use of an angle-dependent rate coefficient to model the effect of particle inertia, while the second made use of a particle *velocity decomposition* that separated the velocity into an inertial part and a diffusive part. We have concluded that the semi-empirical approach cannot lead to an efficient treatment of the filtration problem, and in this study we have directed most of our effort toward the development of the velocity decomposition approach. Problems arise with the velocity decomposition method because the particle tracking equation is hyperbolic in nature, and there are regions in the flow field where it is difficult to calculate the deterministic particle velocity. These problems can be avoided with an asymptotic analysis, and we have used this approach to determine single fiber efficiencies for small Stokes numbers. These efficiencies illustrate a *minimum* as a function of the particle diameter; however, the range of validity (in terms of the Stokes number) of the asymptotic method is uncertain. If the range of validity of the asymptotic expansion is suitable for the solution of practical problems, the current work on *homogeneous filters* should be expanded to include a broader range of values of the key parameters and then extended to include the case of *heterogeneous filters*. If the range of validity of the asymptotic method is not suitable for the solution of practical problems, the particle tracking problem must be resolved or we must move on to the use of *Brownian dynamics*. This approach is outlined in Sec. 1 where we have indicated how Brownian dynamics may be incorporated into the *method of volume averaging*.

1. Introduction

The hierarchical nature of the filtration process is illustrated in Figure 1 where we have indicated that the physics associated with the particle capture process must be *transported* to the filter design scale if we are to be able to analyze and design filters with confidence. The physics of the process consists of the continuity equation and the equation of motion for the particles, along with a consistent representation for the boundary condition at the fluid-solid interface. The continuity equation for the particles in a filtration process can be written as

$$\frac{\partial n_p}{\partial t} + \nabla \cdot (\mathbf{v}_p n_p) = 0, \quad \text{in the } \gamma\text{-phase} \quad (1)$$

in which n_p and $\mathbf{v}_p$ refer to the ensemble average number density and velocity of particles having a specified size p . An acceptable boundary condition for many filtration processes is given by

Figure 1
Hierarchical View of the Filtration Process

$$\text{B.C. 1} \quad n_p = 0, \quad \text{at the } \gamma\text{-}\sigma \text{ interface} \quad (2)$$

and we will use this condition to describe the physics at the surface of the fiber in all of our calculations. Equation 1 is obtained by ensemble averaging the motion of particles obeying the following momentum equation

$$m_p \frac{d\mathbf{V}_p}{dt} = -3\pi\mu d_p (\mathbf{V}_p - \mathbf{v}) + \mathbf{F}_r(t) \quad \text{in the } \gamma\text{-phase} \quad (3)$$

Here m_p is the mass of the particle p , d_p is the particle diameter, and $\mathbf{v}$ is the fluid velocity determined by the Navier-Stokes equations. The first term on the right hand side represents Stokes' law for the drag force and $\mathbf{F}_r(t)$ represents the random or Brownian force. The particle velocity can be decomposed into two parts which are expressed as

$$\mathbf{V}_p = \bar{\mathbf{V}}_p + \mathbf{U}_p \quad (4)$$

We require that the first part satisfy the following deterministic equation

$$m_p \frac{d\bar{\mathbf{V}}_p}{dt} = -3\pi\mu d_p (\bar{\mathbf{V}}_p - \mathbf{v}) \quad (5)$$

and this means that the second part must satisfy the stochastic equation given by

$$m_p \frac{d\mathbf{U}_p}{dt} = -3\pi\mu d_p \mathbf{U}_p + \mathbf{F}_r(t) \quad (6)$$

This is the classic equation of motion for Brownian diffusion and it leads to the representation for the *ensemble average* Brownian velocity, $\mathbf{u}_p$, given by

$$\mathbf{u}_p = -D_p \nabla n_p \quad (7)$$

in which D_p is the Brownian motion diffusivity. This suggests that it is possible to decompose the particle velocity according to

$$\mathbf{V}_p = \bar{\mathbf{V}}_p + \mathbf{u}_p \quad (8)$$

in which $\bar{\mathbf{V}}_p$ is the *ensemble average* value of the particle velocity, $\mathbf{V}_p$, and $\mathbf{u}_p$ is the Brownian velocity given by Eq. 7.

Use of Eqs. 7 and 8 in Eq. 1 provides the following particle transport problem

$$\frac{\partial n_p}{\partial t} + \nabla \cdot (\bar{\mathbf{v}}_p n_p) = \nabla \cdot (D_p \nabla n_p), \quad \text{in the } \gamma\text{-phase} \quad (9)$$

$$\text{B.C. 1} \quad n_p = 0, \quad \text{at the } \gamma\text{-}\sigma \text{ interface} \quad (10)$$

A key problem associated with this approach is the determination of the velocity $\bar{\mathbf{v}}_p$. This requires the solution of a particle tracking equation *and* the interpolation of the computed velocities to obtain values of $\bar{\mathbf{v}}_p$ at the grid points that will be used with the finite difference solution of Eq. 9. To avoid this difficulty, it was originally proposed to modify Eqs. 9 and 10 and replace them with

Case I: The Semi-Empirical Approach.

$$\frac{\partial n_p}{\partial t} + \nabla \cdot (\mathbf{v} n_p) = \nabla \cdot (D_p \nabla n_p) \quad \text{in the } \gamma\text{-phase} \quad (11)$$

$$\text{B.C. 2} \quad -\mathbf{n}_{\gamma\sigma} \cdot D_p \nabla n_p = k_p(\theta) n_p, \quad \text{at the } \gamma\text{-}\sigma \text{ interface} \quad (12)$$

Here $\mathbf{v}$ represents the continuum velocity determined by a numerical solution of the Navier-Stokes equations, and $k_p(\theta)$ represents an empirical rate coefficient which is to be chosen in order to *fit* the observed single fiber behavior determined by Brownian dynamics. In this approach, one solves Eqs. 11 and 12, and uses the results to compute the rate of capture according to

$$\left\{ \begin{array}{l} \text{rate of particle} \\ \text{capture at a} \\ \text{single fiber} \end{array} \right\} = \int_{\theta=0}^{\theta=2\pi} k_p(\theta) n_p a d\theta \quad (13)$$

Here a represents the fiber radius and $k_p(\theta)$ is to be adjusted so that the results of the calculation will *fit* the single fiber efficiency (Tien and Ramarao) illustrated in Figure 2. The original proposal suggested that $k_p(\theta)$ could be *adjusted* as indicated in Figure 3 in order to model the effects of particle inertia and therefore reproduce the minimum illustrated in Figure 2. A little thought will indicate that a *unique* function, $k_p(\theta)$, cannot be extracted from this type of analysis, thus we consider this approach to be unacceptable. The obvious failure of the semi-empirical approach led us to the deterministic particle tracking approach which can be described by

Case II: Deterministic Particle Tracking.

Figure 2
Single Fiber Efficiency

Figure 3
Adsorption Rate Coefficients for Different Particle Sizes

$$\frac{\partial n_p}{\partial t} + \nabla \cdot (\bar{\mathbf{v}}_p n_p) = \nabla \cdot (D_p \nabla n_p), \quad \text{in the } \gamma\text{-phase} \quad (14)$$

$$\text{B.C. 1} \quad n_p = 0, \quad \text{at the } \gamma\text{-}\sigma \text{ interface} \quad (15)$$

The ensemble average velocity $\bar{\mathbf{v}}_p$ is determined by solving the particle momentum equation, Eq. 5, for different initial conditions. Problems associated with this approach are discussed in Sec. 3. An alternative route is based on the key hypothesis that the *ensemble average* velocity $\bar{\mathbf{v}}_p$ obeys the same equation as $\bar{\mathbf{V}}_p$. This hypothesis leads to the following particle tracking equation

$$m_p \frac{d\bar{\mathbf{v}}_p}{dt} = -3\pi\mu d_p (\bar{\mathbf{v}}_p - \mathbf{v}), \quad \text{in the } \gamma\text{-phase} \quad (16)$$

In this approach one first determines $\mathbf{v}$ by a numerical solution of the Navier-Stokes equations, and one then uses Eq. 16 to calculate the deterministic particle velocity, $\bar{\mathbf{v}}_p$. While this seems like a straightforward approach, there are significant problems with the use of Eq. 16 in systems that are representative of fibrous filters, and these will be discussed in the next section.

The problems associated with Eq. 16 can be removed by returning to Eq. 1 and making use of the complete representation of the particle equation of motion. This approach is referred to as Brownian dynamics and it leads to the following formulation of the filtration problem.

Case III: Brownian Dynamics and the Method of Volume Averaging.

In this approach we make use of the particle continuity equation given by

$$\frac{\partial n_p}{\partial t} + \nabla \cdot (\mathbf{v}_p n_p) = 0, \quad \text{in the } \gamma\text{-phase} \quad (17)$$

along with the particle equation of motion

$$m_p \frac{d\mathbf{V}_p}{dt} = -3\pi\mu d_p (\mathbf{V}_p - \mathbf{v}) + \mathbf{F}_r(t) \quad \text{in the } \gamma\text{-phase} \quad (18)$$

and the boundary condition at the surface of a fiber

$$\text{B.C. 1} \quad n_p = 0, \quad \text{at the } \gamma\text{-}\sigma \text{ interface} \quad (19)$$

Here $\mathbf{F}_r(t)$ is the random or Brownian force, and Eq. 18 is used to simulate the motion of particles *in a unit cell* that is representative of a fibrous filter. In order to combine the

method of Brownian dynamics with the method of volume averaging, we form the local volume average of Eq. 17 and make use of the averaging theorem (Howes and Whitaker, 1985) to obtain

$$\epsilon_\gamma \frac{\partial \langle n_p \rangle^\gamma}{\partial t} + \nabla \cdot \langle \mathbf{v}_p n_p \rangle = -\frac{1}{\tau_0} \int_{A_{\gamma\sigma}} \mathbf{n}_{\gamma\sigma} \cdot \mathbf{v}_p n_p dA \quad (20)$$

Here the local volume average concentration of particles is defined explicitly by

$$\langle n_p \rangle^\gamma = \frac{1}{V_\gamma} \int_{V_\gamma} n_p dV \quad (21)$$

in which V_γ is the volume of the gas phase contained within the averaging volume, τ_0 . These two volumes are related by

$$V_\gamma = \epsilon_\gamma \tau_0 \quad (22)$$

and are therefore nearly equal for the typical fibrous filter. Since the filtration process is quasi-steady, the first term in this equation is always negligible; however, it is convenient to retain this term as a reminder that Eq. 20 is the governing differential equation for the volume averaged particle concentration, $\langle n_p \rangle^\gamma$. The term on the right hand side of Eq. 20 is the all important *rate of particle capture per unit volume of the filter* and this is to be determined by a Brownian dynamics simulation. Before that simulation is carried out we need to arrange Eq. 20 in the form of a *transport equation* for $\langle n_p \rangle^\gamma$. We begin that process with the decompositions

$$\mathbf{v}_p = \langle \mathbf{v}_p \rangle^\gamma + \tilde{\mathbf{v}}_p \quad (23a)$$

$$n_p = \langle n_p \rangle^\gamma + \tilde{n}_p \quad (23b)$$

and follow the type of analysis used in the study of dispersion in porous media (Carbonell and Whitaker, 1983) to obtain

$$\epsilon_\gamma \frac{\partial \langle n_p \rangle^\gamma}{\partial t} + \nabla \cdot [\epsilon_\gamma \langle \mathbf{v}_p \rangle^\gamma \langle n_p \rangle^\gamma] + \nabla \cdot \langle \tilde{\mathbf{v}}_p \tilde{n}_p \rangle = -\frac{1}{\tau_0} \int_{A_{\gamma\sigma}} \mathbf{n}_{\gamma\sigma} \cdot \mathbf{v}_p n_p dA \quad (24)$$

This form contains $\langle n_p \rangle^\gamma$ which we would like to predict in order to design a filter or to compare theory with experiment; however, it also contains the *average particle velocity* $\langle \mathbf{v}_p \rangle^\gamma$ and we would prefer to work with the *average fluid velocity*. Because of this we express Eq. 24 as

$$\begin{aligned}
\underbrace{\epsilon_\gamma \frac{\partial \langle n_p \rangle^\gamma}{\partial t}}_{\text{accumulation}} + \underbrace{\nabla \cdot [\epsilon_\gamma \langle \mathbf{v} \rangle^\gamma \langle n_p \rangle^\gamma]}_{\text{traditional convection}} + \underbrace{\nabla \cdot [\epsilon_\gamma (\langle \mathbf{v}_p \rangle^\gamma - \langle \mathbf{v} \rangle^\gamma) \langle n_p \rangle^\gamma]}_{\text{inertial convection}} = \\
\underbrace{-k_{eff} \langle n_p \rangle^\gamma}_{\substack{\text{rate of capture} \\ \text{via Brownian} \\ \text{dynamics}}} - \underbrace{\nabla \cdot \langle \tilde{\mathbf{v}}_p \tilde{n}_p \rangle}_{\text{dispersion}} \quad (25)
\end{aligned}$$

In the classical one-dimensional analysis of a filtration process, Eq. 25 is represented as

$$\epsilon_\gamma \langle v_x \rangle^\gamma \frac{d \langle n_p \rangle^\gamma}{dx} = -k_{eff} \langle n_p \rangle^\gamma \quad (26)$$

in which the product $\epsilon_\gamma \langle v_x \rangle^\gamma$ is the superficial velocity determined as the volumetric flow rate divided by the cross sectional area of the filter. We are certain that the accumulation term in Eq. 25 can be neglected; however, the inertial convection and the dispersion terms should be considered before one accepts Eq. 26 as a reliable representation of the filtration process.

Certainly the key issue in Eq. 25 is the determination of k_{eff} which is defined by

$$k_{eff} = \left(\frac{1}{\langle n_p \rangle^\gamma} \right) \frac{1}{\mathcal{V}} \int_{A_{\gamma\sigma}} \mathbf{n}_{\gamma\sigma} \cdot \mathbf{v}_p n_p dA \quad (27)$$

and which is be calculated by Brownian dynamics for any representative unit cell. The use of Brownian dynamics in a unit cell *to simulate a steady-state, spatially periodic filtration process* requires some thought; however, the approach seems quite feasible. Since part of the Brownian dynamics calculation requires the solution of the Navier-Stokes equations to produce the fluid velocity, $\mathbf{v}$, one can also determine the *inertial convection* term in Eq. 25 in order to assess the importance of this transport mechanism.

2. Velocity Decomposition

The problem under consideration is represented by Eqs. 17 through 19 which we repeat here as

$$\frac{\partial n_p}{\partial t} + \nabla \cdot (\mathbf{v}_p n_p) = 0, \quad \text{in the } \gamma\text{-phase} \quad (28)$$

$$m_p \frac{d\mathbf{V}_p}{dt} = -3\pi\mu d_p (\mathbf{V}_p - \mathbf{v}) + \mathbf{F}_r(t), \quad \text{in the } \gamma\text{-phase} \quad (29)$$

$$\text{B.C. 1} \quad n_p = 0, \quad \text{at the } \gamma\text{-}\sigma \text{ interface} \quad (30)$$

Our goal is to develop a theory, based on these equations, that can predict the behavior of a filter such as the one illustrated in Figure 1. In the velocity decomposition method, we decompose the velocity according to

$$\mathbf{v}_p = \bar{\mathbf{v}}_p + \mathbf{u}_p \quad (31)$$

in which $\bar{\mathbf{v}}_p$ represents the ensemble average velocity associated with the deterministic momentum equation and $\mathbf{u}_p$ represents the contribution due to the Brownian or random forces acting on the particle. We require that the "deterministic" part, $\bar{\mathbf{v}}_p$, satisfy the following particle tracking equation

$$m_p \frac{d\bar{\mathbf{v}}_p}{dt} = -3\pi\mu d_p (\bar{\mathbf{v}}_p - \mathbf{v}) \quad (32)$$

and on the basis of Eqs. 29, 31, and 32, we see that the random part, $\mathbf{u}_p$, is an ensemble average velocity associated with the following equation of motion

$$m_p \frac{d\mathbf{U}_p}{dt} = -3\pi\mu d_p \mathbf{U}_p + \mathbf{F}_r(t) \quad (33)$$

This represents the classical equation for the motion of a Brownian particle in a quiescent fluid (Russel, 1981), thus we know that $\mathbf{u}_p$ is given by

$$\mathbf{u}_p = -D_p \nabla n_p \quad (34)$$

provided that the effects of initial conditions can be ignored. We now return to the particle continuity equation given by Eq. 28 and make use of Eqs. 31 and 33 to obtain

$$\frac{\partial n_p}{\partial t} + \nabla \cdot (\bar{\mathbf{v}}_p n_p) = \nabla \cdot (D_p \nabla n_p) \quad (35)$$

This equation is to be solved subject to the boundary condition given by Eq. 30 and with $\bar{\mathbf{v}}_p$ determined by Eq. 32. By "solved" we mean that the volume averaged form of Eq. 35 needs to be developed and the coefficients in that volume averaged transport equation need to be determined. We form the volume averaged of Eq. 35 and follow the type of analysis indicated by Eqs. 20 through 25 to eventually arrive at

$$\begin{aligned}
\underbrace{\varepsilon_\gamma \frac{\partial \langle n_p \rangle^\gamma}{\partial t}}_{\text{accumulation}} + \underbrace{\nabla \cdot (\varepsilon_\gamma \langle \bar{\mathbf{v}}_p \rangle^\gamma \langle n_p \rangle^\gamma)}_{\text{convection}} = \\
\underbrace{\nabla \cdot \left[\varepsilon_\gamma D_p \left(\nabla \langle n_p \rangle^\gamma + \frac{1}{V_\gamma} \int_{A_{\gamma\sigma}} \mathbf{n}_{\gamma\sigma} \tilde{n}_p dA \right) \right]}_{\text{diffusion}} - \underbrace{\nabla \cdot \langle \tilde{\mathbf{v}}_p \tilde{n}_p \rangle}_{\text{dispersion}} + \underbrace{\frac{1}{V} \int_{A_{\gamma\sigma}} \mathbf{n}_{\gamma\sigma} \cdot D_p \nabla \tilde{n}_p dA}_{\text{particle capture}} \quad (36)
\end{aligned}$$

Here we must be careful to note that the velocity deviation, $\tilde{\mathbf{v}}_p$ is defined according to

$$\bar{\mathbf{v}}_p = \langle \bar{\mathbf{v}}_p \rangle^\gamma + \tilde{\mathbf{v}}_p \quad (37)$$

and is therefore different from $\tilde{\mathbf{v}}_p$ as defined by Eq.23a. The details of the volume averaging procedure are too complicated to present here; however, they can be found in papers by Carbonell and Whitaker (1984), Zanotti and Carbonell (1984), and Quintard and Whitaker (1993).

In Eq. 36 we are confronted with a *closure problem*, i.e., we need to determine $\tilde{\mathbf{v}}_p$ and $\tilde{n}_p$ in order to obtain a *closed form* transport equation that can be used to predict values of $\langle n_p \rangle^\gamma$. The development of the closure problem is much too long to be given here and the interested reader is referred to the references cited above. The closed form of Eq. 36 can be expressed as

$$\begin{aligned}
\varepsilon_\gamma \frac{\partial \langle n_p \rangle^\gamma}{\partial t} + \langle \mathbf{v} \rangle \cdot \nabla \langle n_p \rangle^\gamma + \nabla \cdot \left[\varepsilon_\gamma (\langle \bar{\mathbf{v}}_p \rangle^\gamma - \langle \mathbf{v} \rangle^\gamma) \langle n_p \rangle^\gamma \right] - (\mathbf{u}_\gamma + \mathbf{d}_\gamma) \cdot \nabla \langle n_p \rangle^\gamma \\
= \nabla \cdot (\mathbf{D}^* \cdot \nabla \langle n_p \rangle^\gamma) - k_{eff} \langle n_p \rangle^\gamma \quad (38)
\end{aligned}$$

in which $\langle \mathbf{v} \rangle$ represents the superficial fluid velocity. The coefficients $\mathbf{u}_\gamma$, $\mathbf{d}_\gamma$, $\mathbf{D}^*$, and k_{eff} are determined by the solution of two closure problems that are given by

PROBLEM I

$$\nabla \cdot (\bar{\mathbf{v}}_p \mathbf{b}) + \tilde{\tilde{\mathbf{v}}}_p = \nabla \cdot (D_p \nabla \mathbf{b}) - \epsilon_\gamma^{-1} \frac{1}{\mathcal{V}} \int_{A_{\gamma\sigma}} \mathbf{n}_{\gamma\sigma} \cdot D_p \nabla \mathbf{b} dA \quad (39a)$$

$$\text{B.C. 1} \quad \mathbf{b} = 0, \text{ at the } \gamma\text{-}\sigma \text{ interface} \quad (39b)$$

$$\text{Periodicity:} \quad \mathbf{b}(\mathbf{r} + \ell_i) = \mathbf{b}(\mathbf{r}), \quad i = 1, 2, 3 \quad (39c)$$

$$\text{Average:} \quad \langle \mathbf{b} \rangle_\gamma = 0 \quad (39d)$$

PROBLEM II

$$\nabla \cdot (\bar{\mathbf{v}}_p s) - \nabla \cdot \tilde{\tilde{\mathbf{v}}}_p = \nabla \cdot (D_p \nabla s) - \epsilon_\gamma^{-1} \frac{1}{\mathcal{V}} \int_{A_{\gamma\sigma}} \mathbf{n}_{\gamma\sigma} \cdot D_p \nabla s dA \quad (40a)$$

$$\text{B.C. 1} \quad s = 1, \quad \text{at the } \gamma\text{-}\sigma \text{ interface} \quad (40b)$$

$$\text{Periodicity:} \quad s(\mathbf{r} + \ell_i) = s(\mathbf{r}) \quad (40c)$$

$$\text{Average:} \quad \langle s \rangle_\gamma = 0 \quad (40d)$$

After these closure problems are solved, one can compute the coefficients in Eq. 36 according to the following formulas.

$$\mathbf{u}_\gamma = \frac{1}{\mathcal{V}} \int_{A_{\gamma\sigma}} \mathbf{n}_{\gamma\sigma} \cdot D_p \nabla \mathbf{b} dA \quad (41)$$

$$\mathbf{d}_\gamma = -D_p \left[\frac{1}{\mathcal{V}} \int_{A_{\gamma\sigma}} \mathbf{n}_{\gamma\sigma} s dA \right] + \langle \tilde{\tilde{\mathbf{v}}}_p s \rangle \quad (42)$$

$$\mathbf{D}^* = D_p \left[\epsilon_\gamma \mathbf{I} + \frac{1}{\mathcal{V}} \int_{A_{\gamma\sigma}} \mathbf{n}_{\gamma\sigma} \mathbf{b} dA \right] - \langle \tilde{\tilde{\mathbf{v}}}_p \mathbf{b} \rangle \quad (43)$$

$$k_{eff} = \frac{1}{\mathcal{V}} \int_{A_{\gamma\sigma}} \mathbf{n}_{\gamma\sigma} \cdot D_p \nabla s dA \quad (44)$$

In order to solve Eqs 39 and 40 so that the coefficients given by Eqs. 41 through 44 can be determined, one needs to calculate $\mathbf{v}$ from the Navier-Stokes equations and $\bar{\mathbf{v}}_p$ from the particle tracking equation given by Eq. 32. Given these two velocity fields we can calculate both the average values and the spatial deviation velocity defined by Eq. 37. In the next section we discuss the velocity field calculations and then we will move on to the prediction of the coefficients that appear in the volume averaged transport equation for $\langle n_p \rangle^Y$.

3. Determination of Velocity Fields

The simplest model of a fibrous porous medium is a regular array of cylinders such as that shown in Figure 4. For most practical cases, the Reynolds number for flow in fibrous filters is less than one, thus one can use the Stokes equations to determine the fluid velocity profile. This means that the fluid mechanical problem to be solved is given by

$$\nabla \cdot \mathbf{v} = 0 \quad (45)$$

$$0 = -\nabla p + \rho \mathbf{g} + \mu \nabla^2 \mathbf{v} \quad (46)$$

$$\text{Periodicity:} \quad \mathbf{v}(\mathbf{r} + \ell_i) = \mathbf{v}(\mathbf{r}), \quad i = 1, 2, \text{ and } 3 \quad (47)$$

and the dimensionless velocity profile ($v_x / \langle v_x \rangle^Y$ as a function of y) at the entrance of a unit cell is illustrated in Figure 5. There we see that the velocity profile is not uniform as is commonly assumed in various particle tracking calculations associated with the determination of single fiber efficiencies. The center of the cell associated with the profile shown in Figure 5 is at $y/\ell_y = 0.5$, thus we see that the *entrance velocity* at the *edge* of the cell is about twice as large as the velocity at the *center* of the cell.

Given the fluid velocity field calculated on the basis of Eqs. 45 through 47, one can calculate the deterministic particle velocity, $\bar{\mathbf{v}}_p$, from Eq. 5 and several particle trajectories are shown in Figure 6 for a Stokes number of 0.0155. In this case the Stokes number is defined by

$$St = \frac{\langle v_x \rangle^Y \rho_p d_p^2}{18\mu \ell_y} \quad (48)$$

in which ρ_p is the particle density and d_p is the particle diameter. The Stokes number given by Eq. 48 involves the characteristic length of a unit cell, ℓ_y , and is thus different than other definitions of the Stokes number that are available in the literature. For the first unit cell shown in Figure 6 there is a wake region that contains no particle trajectories, and

Figure 4
Spatially Periodic Array of Cylinders

Figure 5
Velocity Profile at the Entrance of a Unit Cell

Figure 6
Particle Trajectories in a Spatially Periodic Porous Medium

for subsequent unit cells there is an "upstream region" that is also devoid of trajectories. We will refer to these two regions as "dead regions" in order to indicate that they are not accessible by *straightforward* particle trajectory calculations. This does not mean that there are no particles in these two regions nor does it mean the particle trajectories cannot be calculated in these two regions. What it does mean is that the determination of $\bar{v}_p$ everywhere represents an *unsolved problem* that requires a careful treatment of the boundary condition for $\bar{v}_p$ on the downstream side of the fiber.

The characteristic of the particle trajectories that is most interesting is the evolution of the $\bar{v}_p$ -field which is illustrated in Figure 7. There the dimensionless x-component of $\bar{v}_p$ is shown for several Stokes numbers, and for a Stokes number of 0.155 we see that approximately ten cells are required before a stationary state is reached. From Figure 5 we know that the fluid velocity is not uniform at the entrance of a unit cell, and when we add the dimensionless x-component of $\bar{v}_p$ to Figure 5 we obtain the comparison between v and $\bar{v}_p$ shown in Figure 8. There we see the fluid velocity profile calculated on the basis of Eqs. 45 through 47 along with points obtained from the solution of the particle tracking equation given earlier by Eq. 5 as listed here for convenience as

$$m_p \frac{d\bar{v}_p}{dt} = -3\pi\mu d_p (\bar{v}_p - v), \quad \text{particle tracking equation} \quad (49)$$

The results presented in Figure 8 for the particle velocities show the absence of particle trajectories in the upstream portion of the "dead region." Particle trajectories are readily available in this region for the *first unit cell*; however, after the first unit cell there are no particle trajectories in either the upstream or the downstream portions of the "dead region." Again we note that this does not mean that values of $\bar{v}_p$ do not exist in the "dead region", it simply means that one must develop a separate solution of Eq. 49 in the wake of a cylinder using an appropriate boundary condition at the downstream surface of the cylinder. Once the $\bar{v}_p$ -field is known in the wake region, one can invoke periodicity to determine $\bar{v}_p$ at the entrance of the upstream portion of the "dead region" and then solve Eq. 49 in the normal manner in order to produce the entire $\bar{v}_p$ -field. At this time we have not explored the problem of an appropriate boundary condition for $\bar{v}_p$ at the downstream side of a cylinder; however, it is clear that one can set $\bar{v}_p$ equal to v close to the solid surface over much, *but not all*, of the wake region.

ASYMPTOTIC APPROXIMATION

In order to circumvent the difficulties associated with the particle tracking equation, one can develop an approximate solution for the ensemble average deterministic velocity $\bar{v}_p$ using the asymptotic method first presented by Yeh and Liu (1974) and later used by Banks and Kurowski (1983). To illustrate this procedure, we express Eq. 32 in dimensionless form according to

Figure 7
Evolution of the Particle Trajectories

Figure 8
Comparison of Fluid Velocity and Particle Velocities at the Entrance of a Unit Cell

$$St \frac{d\bar{\mathbf{v}}_p^*}{dt^*} = -(\bar{\mathbf{v}}_p^* - \mathbf{v}^*) \quad (50)$$

and assume an expansion of the form

$$\bar{\mathbf{v}}_p^* = \bar{\mathbf{v}}_p^0 + St \bar{\mathbf{v}}_p^1 + St^2 \bar{\mathbf{v}}_p^2 + \dots \quad (51)$$

Use of Eq. 51 in Eq. 50 and equating the coefficients of like powers of the Stokes number leads to

$$\bar{\mathbf{v}}_p^0 = \mathbf{v}^* \quad (52a)$$

$$\bar{\mathbf{v}}_p^1 = -\frac{d\bar{\mathbf{v}}_p^0}{dt^*} \quad (52b)$$

$$\bar{\mathbf{v}}_p^2 = 0 \quad (52c)$$

The time derivative in Eq. 48b can now be written as

$$\frac{d\bar{\mathbf{v}}_p^0}{dt^*} = \bar{\mathbf{v}}_p^0 \cdot \nabla \mathbf{v}^* \quad (53)$$

and when this result is used in Eq. 47 along with Eqs. 52a and 52b we find that the dimensionless deterministic particle velocity is given by

$$\bar{\mathbf{v}}_p^* = \mathbf{v}^* - St \mathbf{v}^* \cdot \nabla \mathbf{v}^* \quad (54)$$

In this case one need only solve the fluid mechanics problem represented by Eqs. 45 through 47 in order to determine the deterministic part of the particle velocity. In addition, one can use Eq. 54 to determine $\bar{\mathbf{v}}_p^*$ everywhere so that the "dead region" encountered with the direct particle tracking calculations is no longer a problem. In the next section we present results for the effective coefficients in Eq. 38 making use of Eq. 54.

4. Effective Coefficients in the Volume Averaged Particle Transport Equation

We are now ready to return to Eq. 38 and to examine the various terms in that volume averaged particle transport equation. The first term in Eq. 38 represents the accumulation in the gas phase and in general this term is zero for a wide range of practical

problems. The next term, $\langle \mathbf{v} \rangle \cdot \nabla \langle n_p \rangle^\gamma$, represents the convective transport which is usually set equal to the last term in Eq. 38 to obtain

$$\langle v_x \rangle \frac{d\langle n_p \rangle^\gamma}{dx} = -k_{eff} \langle n_p \rangle^\gamma \quad (55)$$

however, before examining the nature of k_{eff} , we need to consider the other terms in Eq. 38. While the deterministic particle velocity, $\bar{\mathbf{v}}_p$, is clearly different from the fluid velocity, $\mathbf{v}$, the average values represented by $\langle \bar{\mathbf{v}}_p \rangle^\gamma$ and $\langle \mathbf{v} \rangle^\gamma$ are very close to each other *provided* that one uses the asymptotic representation given by Eq. 54 to calculate $\bar{\mathbf{v}}_p$. If this is also true for the exact representation of $\bar{\mathbf{v}}_p$, the third term in Eq. 38 could be neglected. The fourth term in Eq. 38 involves the two coefficients, $\mathbf{u}_\gamma$ and $\mathbf{d}_\gamma$, that are determined by the solution of the two closure problems given by Eqs. 39 and 40. Calculated values of the x-components of $\mathbf{u}_\gamma$ and $\mathbf{d}_\gamma$, made dimensionless by $\langle v_x \rangle$, are shown in Figures 9 as a function of the interstitial fluid velocity for the following conditions

$$\begin{aligned} d_p &= 0.5 \text{ and } 0.1 \quad \mu\text{m} \\ \rho_p &= 4.0 \quad \text{g/cm}^3 \\ T &= 283.0 \quad \text{K} \\ \mu &= 1.8 \times 10^{-5} \quad \text{Pa s} \\ \varepsilon_\gamma &= 0.95 \end{aligned}$$

The results presented in Figures 9 indicate that $\mathbf{u}_\gamma$ and $\mathbf{d}_\gamma$ provide a contribution to the convective transport that is non-negligible. The values for a Stokes number of zero represent the purely diffusive case and the increase in the convective transport occurs because the slow moving particles near the solid surface are removed thus leading to a larger overall velocity. For the finite Stokes numbers associated with the conditions listed above, we see that the *sign of the effect changes* for a velocity of about 0.05 m/s for $d_p = 0.1 \mu\text{m}$ and for a velocity of about 0.01 m/s for $d_p = 0.5 \mu\text{m}$. For the larger particle size the *effect itself becomes very significant* when the fluid velocity is greater than 0.01 m/s. The diminished convective transport at larger Stokes numbers presumably results from the fact that the high velocity particles are more effectively removed by inertial capture and this leads to a reduced convective transport. At the highest velocity represented in Figure 9b, we see an abrupt change in the behavior of $\mathbf{u}_\gamma$ and $\mathbf{d}_\gamma$ and this may be due to numerical difficulties or due to the fact that the asymptotic representation given by Eq. 54 is not accurate at the larger Stokes numbers.

Moving on to the right hand side of Eq. 38, we encounter the dispersive contribution to the particle transport. In general, one can neglect dispersive transport relative to convective transport for one-dimensional transport processes; however, the particle transport equation given by Eq. 38 represents a transport equation for *homogeneous* filters and when it is later used to develop a theory for *heterogeneous* filters

Figure 9a
Velocity Coefficients as a Function of the Interstitial Fluid Velocity
($d_p = 0.1 \mu\text{m}$, $2a = 0.1 \mu\text{m}$)

Figure 9b
Velocity Coefficients as a Function of the Interstitial Fluid Velocity
($d_p = 0.5 \mu\text{m}$, $2a = 0.5 \mu\text{m}$)

the dispersive transport may play an important role. Calculated results for the longitudinal dispersion coefficient made dimensionless by the Brownian diffusivity are shown in Figures 10 for two different particle sizes. Once again the case for $St = 0$ represents the diffusive case and the results are representative of the original calculations of Eidsath et al (1983). For the finite Stokes numbers the dispersion coefficient diminishes slightly at the higher velocities for $d_p = 0.5 \mu m$ and no influence of particle inertia is seen for $d_p = 0.1 \mu m$. The results shown in Figures 10 suggest that the classical dispersion coefficients obtained for species having negligible inertia represent an upperbound for the longitudinal dispersion of aerosol particles.

CELLULAR EFFICIENCY

In the previous paragraphs we have presented results for the coefficients that appear in the volume average particle transport equation given by Eq. 38. The accumulation and dispersion terms may be neglected with some confidence, while questions about the importance of the non-traditional convective transport terms remain. In order to present our results for k_{eff} in a traditional form, we will simplify Eq. 38 to Eq. 55 and solve that equation to represent the change in particle concentration that takes place across a unit cell as

$$\frac{\langle n_p \rangle^\gamma \Big|_{x=0} - \langle n_p \rangle^\gamma \Big|_{x=\ell_y}}{\langle n_p \rangle^\gamma \Big|_{x=0}} = 1 - e^{-\frac{k_{eff} \ell_y}{\langle v_x \rangle}} \quad (56)$$

It is convenient to define the left hand side of this result as the *cellular efficiency*, η_c , in order to distinguish it from the *single fiber efficiency*, and this leads to

$$\eta_c = 1 - e^{-\frac{k_{eff} \ell_y}{\langle v_x \rangle}} \quad (57)$$

Values for η_c are shown in Figure 11 as a function of the particle diameter. The curve for $St = 0$ represents the purely diffusive case and does not exhibit a minimum. The curve for finite Stokes numbers, which range from 10^{-4} to almost 10^{-1} , indicate a minimum cellular efficiency for particle diameters on the order of 1 to 2 micrometers. While this type of behavior is in reasonable agreement with the Brownian dynamics of Tien and Ramarao we cannot make a meaningful comparison without knowing the particle density.

In thinking about the results shown in Figure 11, one must be careful to remember the additional convective transport represented by the coefficients u_y and d_y . The magnitude of these non-traditional terms is represented in Figures 9a and 9b where we see contributions to the "velocity" on the order of 10%. Given the uncertainty in many parts of the analysis, one might be inclined to ignore an effect of 10%; however, an increase of 10% in the velocity $\langle v_x \rangle$ can have an important effect in the exponential function that determines the cellular efficiency given by Eq. 57.

Figure 10a
Longitudinal Dispersion Coefficients

($d_p = 0.5 \mu\text{m}$, $2a = 0.5 \mu\text{m}$, $\rho_p = 4000 \text{ kg/m}^3$
 $T = 283 \text{ K}$, $\mu = 1.8 \cdot 10^{-5} \text{ Pa s}$, $\epsilon_p = 0.95$)

Figure 10b
Longitudinal Dispersion Coefficients

($d_p = 0.1 \mu\text{m}$, $2a = 0.1 \mu\text{m}$, $\rho_p = 4000 \text{ kg/m}^3$
 $T = 283 \text{ K}$, $\mu = 1.8 \cdot 10^{-5} \text{ Pa s}$, $\epsilon_p = 0.95$)

Figure 11
Cellular Efficiency as a Function of Particle Diameter

($2a = 0.5 \mu\text{m}$, $\rho_p = 4000 \text{ kg/m}^3$
 $T = 283 \text{ K}$, $\mu = 1.8 \cdot 10^{-5} \text{ Pa s}$, $\epsilon_g = 0.95$)

5. Conclusions

In this work we have discussed (briefly) an empirical approach to the problem of particle inertia in the filtration process, and concluded that it is not an effective approach to use in the design and analysis of fibrous filters. The use of Brownian dynamics with the method of volume averaging has been described, but no detailed calculations have been carried out. The coupling of Brownian dynamics with the method of volume averaging represents an entirely new research problem that definitely should be explored in detail. Our main effort in this research project consisted of the use of a velocity decomposition in order to separate the particle transport into a convective-diffusion equation and a deterministic particle tracking equation. The particle tracking equation leads to "dead regions" when employed in the traditional manner, and this difficulty can be circumvented by the use of an asymptotic expansion for the deterministic particle velocity. These results have been used, along with the method of volume averaging, to produce a local volume averaged transport equation for the particle concentration. This equation contains a non-traditional convective transport mechanism which should not be neglected in the design and analysis of filters. From the particle transport equation, one can obtain a cellular efficiency that exhibits a minimum as a function of the particle diameter. If the domain of validity of the asymptotic representation for the deterministic particle velocity is representative of conditions encountered in practical problems, this approach can be extended to heterogeneous filters in order to achieve a reliable method of design and analysis.

6. Nomenclature

Roman Letters

a	fiber radius, m.
$A_{\gamma\sigma}$	area of the γ - σ interface contained within the averaging volume, m^2 .
$\mathbf{b}$	a closure variable, m.
d_p	particle diameter, m.
$\mathbf{d}_\gamma$	a velocity-like coefficient, m/s
D_p	Brownian diffusivity, m^2/s .
$\mathbf{D}^*$	dispersion tensor, m^2/s
$\mathbf{F}_r(t)$	Brownian or random force, N.
$\mathbf{g}$	gravity vector, m/s^2
$k_p(\theta)$	empirical rate coefficient, s^{-1}
k_{eff}	effective rate coefficient for particle capture, s^{-1}
ℓ_γ	characteristic length for a unit cell, m.
ℓ_i	$i = 1, 2, \text{ and } 3$, lattice vectors, m.

m_p	mass of a particle, kg.
n_p	particle density, number/m ³ .
$\langle n_p \rangle^\gamma$	intrinsic average particle concentration, number/m ³ .
$\mathbf{n}_{\gamma\sigma}$	unit normal vector pointing from the γ -phase toward the σ -phase.
p	fluid pressure, N/m ² .
$\mathbf{r}$	position vector, m.
s	a closure variable.
St	$\langle v_x \rangle^\gamma \rho_p d_p^2 / 18\mu \ell_\beta$, the Stokes number.
t	time, s.
$\mathbf{u}_p$	ensemble average Brownian particle velocity, m/s.
$\mathbf{U}_p$	ensemble average Brownian particle velocity, m/s.
$\mathbf{u}_\gamma$	a velocity-like coefficient, m/s.
$\mathbf{v}$	fluid velocity vector, m/s.
$\mathbf{v}^*$	$\mathbf{v} / \langle v_x \rangle^\gamma$, dimensionless fluid velocity.
$\langle \mathbf{v} \rangle^\gamma$	intrinsic average fluid velocity, m/s.
$\tilde{\mathbf{v}}$	$\mathbf{v} - \langle \mathbf{v} \rangle^\gamma$, spatial deviation fluid velocity, m/s.
$\bar{\mathbf{v}}_p$	ensemble average deterministic particle velocity, m/s.
$\bar{\mathbf{V}}_p$	deterministic particle velocity, m/s.
$\bar{\mathbf{v}}_p^*$	$\bar{\mathbf{v}}_p / \langle v_x \rangle^\gamma$, dimensionless deterministic particle velocity.
$\langle \bar{\mathbf{v}}_p \rangle^\gamma$	intrinsic average of the deterministic particle velocity, m/s.
V_γ	volume of the γ -phase contained within the averaging volume, $\mathcal{V}$, m ³ .
$\mathcal{V}$	averaging volume, m ³ .

Greek Letters

μ	fluid viscosity, Ns/m ² .
π	3.1416.....
ϵ_γ	porosity.
ρ	fluid density, kg/m ³ .
ρ_p	particle density, kg/m ³ .

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