CLARIFICATION OF CLEAN-BED FILTRATION MODELS


ABSTRACT: Clean-bed filtration models are frequently used to make engineering calculations on aquasol removal in filters. They consist of a filtration equation, derived from a mass balance around a collector, a single-collector collision efficiency, and an empirically derived sticking coefficient. In order to be correctly applied and referenced, the two most commonly used models, the Yao model and the Rajagopalan and Tien (RT) model, require additional clarification. The filtration equation used in the Yao model has a different form than that of an aerosol counterpart due to assumptions made in choosing a reference velocity in the system. The RT model, as originally published, had variables hidden within constants and contained typographic errors. In this paper we identify the differences in the Yao and aerosol filtration model derivations, correctly present the RT model, and compare model predictions with particle removals reported in laboratory columns.

INTRODUCTION

The filtration model of Yao et al. (1971) has been used to understand and predict particle removal in packed beds, transport of bacteria in ground waters, and feeding by aquatic organisms (Rubenstein and Koech 1977; McDowell-Boyier et al. 1986; Elmelich and O'Melia 1990; Bales et al. 1991; Harvey and Garabedian 1991; Hurst 1991). The model was formulated by applying theoretical solutions of particle removal by an isolated collector in an infinite medium to particle removal in a clean packed bed (i.e., prior to any significant particle accumulation on the collector). It is generally accepted that this model underestimates the number of collisions occurring in packed beds (Bouwer and Rittmann 1992). More recent models, such as the one proposed by Rajagopalan and Tien (RT) (Rajagopalan and Tien 1976; Tien 1989), better account for flow restrictions due to neighboring collectors in packed beds using an approach pioneered by Happel (1958). Both the Yao and RT models continue to be used in many applications.

Due to the importance of filtration theory for describing environmental engineering processes, the main purpose of the present paper is to clarify several aspects of these models to ensure that they are correctly applied to filtration calculations. For example, the filtration equation derived by Yao et al. (1971) to predict aquasol removal has a different mathematical form than its counterpart in aerosol science (Flagen and Seinfeld 1988), although they are both based on similar mass balances. As is shown, the differences in the Yao and aerosol filtration equations can be attributed to assumptions made in choosing a reference velocity for the system. One problem that has arisen with the RT model is that the governing equations presented in the original paper by Rajagopalan and Tien had hidden variables in “constant” terms and contained typographical errors. These errors have gone unnoticed in some investigations, propagating the use of incorrect filtration equations. To avoid further confusion, we clarify the problems with the original Rajagopalan and Tien equations and present the correct forms of the collision and filtration equations.

MODELS OF PARTICLE TRANSPORT

Comparison of Yao and Pore Velocity Filtration Equations

Yao et al. (1971) developed their filtration equation using a mass balance based on particle removal by an isolated sphere, assuming a packed bed is an assemblage of isolated spheres. This equation, referred to here as the Yao model filtration equation, was

\[
\frac{C}{C_0} = \exp \left( -\frac{3}{2} \frac{(1 - \theta)}{d_i} \alpha \eta L \right)
\]

(1)

where \(C_0\) and \(C\) = influent and effluent particle concentrations; \(\theta\) = bed porosity, \(d_i = \) diameter of the spherical collector; \(\alpha = \) sticking coefficient defined as the ratio of the rate particles stick to a collector to the rate they strike the collector; \(\eta = \) single collector collision efficiency; and \(L = \) length of the column.

Eq. 1 is not the only possible solution from a mass balance. For a collector in a packed bed, the same mass-balance approach can be used to derive a steady-state filtration equation,

\[
\frac{C}{C_0} = \exp \left( -\frac{3}{2} \frac{(1 - \theta)}{d_i \theta} \alpha \eta L \right)
\]

(2)

referred to here as the pore velocity (PV) filtration equation. Comparison of the two results shows that these equations differ by a factor of \(\theta\) in the denominator of the right-hand term. This difference results from the selection of a characteristic velocity for the mass balance. The implication of this choice on the final form of the filtration equation can be understood by following a detailed derivation of (2).

From a mass balance across a layer in a packed bed (Fig. 1), the number of particles entering the control volume during a time \(\Delta t\) is \(c_i(A\theta)u\Delta t\), where \(c_i = \) number concentration of particles entering into the control volume \(\Delta V^r\) of thickness \(\Delta z\) and cross-sectional area \(A\), and \(u = \) interstitial or pore velocity. The parentheses around the \((A\theta)\) term are used to emphasize that the porosity reduces the cross-sectional area of flow. Similarly, the rate at which particles are added by modification is \(-D(A\theta)\Delta t(\Delta c_i /\Delta z)\). The rates of advection and dispersion out of the control volume are \(c_i + \Delta t, (A\theta)u\Delta z\) and \(D(A\theta)\Delta t(\Delta c_i + \Delta z /\Delta z)\), respectively.

The removal of particles by collectors is calculated by determining particle accumulation on filter media \(a_s\) as

\[
a_s = r_s \alpha N \Delta t
\]

(3)

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where \( N_c \) = number of collectors in the control volume; and \( r_c \) = the rate particles strike a collector. The number of collectors in the control volume is

\[
N_c = \frac{A(1 - \theta)\Delta z}{\pi d_i^2}
\]

Calculation of \( r_c \) is based on the definition of the single media collector efficiency \( \eta \) defined as

\[
\eta = \frac{r_f}{r_c}
\]

where \( r_f \) = the rate particles flow toward the collector.

The derivations of (1) and (2) differ in the definition of \( r_c \). In the Yao model, \( r_c \) is calculated for an isolated collector and as a consequence is based on the superficial, or approach velocity \( U = u \theta \). However, the superficial velocity does not exist within a packed bed, since adjacent collectors constrict the flow path and increase the fluid velocity around a collector. Therefore, an alternative is to define the characteristic velocity as the pore velocity and calculate \( r_c \) as

\[
r_c = \eta u c \frac{\pi}{4} d_i^2
\]

Except for the choice of the velocity used in calculating \( r_c \), other aspects of the derivation of (2) are identical. Substitution of (4) and (6) into (3), yields

\[
a_c = \frac{3\alpha c(1 - \theta)k\Delta z\Delta t}{2d_i}
\]

Including a term for accumulation in the fluid \( (\Delta c(\Delta t)\Delta z) \) and dividing by \( A \Delta z \Delta t \), the mass balance over the control volume becomes

\[
-\theta \Delta c
\frac{c_i + \Delta c}{\Delta z} + D \left( \frac{\partial^2 c}{\partial z^2} - \frac{\partial c}{\partial z} \right) = \theta \frac{\Delta c}{\Delta t} + \frac{3}{2d_i} \left( 1 - \theta \right) \alpha \eta c u
\]

Taking the limit as \( \Delta z \) and \( \Delta t \) go to zero, and dividing by \( \theta \), produces

\[
- u \frac{\partial c}{\partial z} + D \frac{\partial^2 c}{\partial z^2} = \frac{\partial c}{\partial t} + \frac{3}{2d_i} \left( 1 - \theta \right) \alpha \eta c u
\]

If we neglect dispersion and accumulation in the fluid, (9) becomes

\[
\frac{dc}{dz} = -\frac{3}{2} \left( 1 - \theta \right) \alpha \eta c
\]

Integrating over the length of the column \( L \) yields the PV filtration equation based on the pore velocity in a packed bed (\( \Delta \)). This derivation is in agreement with the solution for aerosol filtration in packed beds made by others (Flagen and Seinfeld 1988). For aerosol-filtration calculations the differences between the two models are negligible, since bed porosities are very close to unity (\( \theta \approx 1 \)).

**Single Collector Efficiencies Calculated Using Yao and PV Model**

There are a variety of analytical solutions that have been developed to specify the collector efficiency for aerosols and aquasols (Logan et al. 1993). For aquasols, Yao et al. (1971) proposed that

\[
\eta = 4N_c^2 u^3 + \frac{3}{2} N_c^2 + N_G
\]

The three terms on the right-hand side indicate removal by diffusion, interception, and gravitational sedimentation, respectively, expressed as a function of three dimensionless numbers, the Peclet number \( N_P = u^* d_i/D_p \), the interception number \( N_I = d_i/d_a \), and the gravitation number \( N_G = U_p/u^* \), where \( D_p \) is the particle diffusion coefficient, \( d_i \) the particle diameter, and \( U_p = g(p_p - p_i)d_i^2/18 \mu \) the particle settling velocity, where \( g \) is the gravitational constant, \( p_i \) the particle density, \( \mu \) the fluid density, and \( \mu \) the fluid viscosity.

The characteristic velocity \( u^* \) is explicitly defined in (11) as the upstream (approach) velocity to the collector. Particle collisions generated by Brownian motion are calculated using a Peclet number based on the analytical solution of Levich (1962) for a sphere in an infinite fluid. For the Levich solution for an isolated sphere to be consistent with the mass balance for an isolated sphere, the approach velocity must be defined as \( u^* = u \theta \). However, the approach velocity does not exist within the packed bed (due to the proximity of other collectors); for a collector in a packed bed, the average velocity of the fluid approaching the collector is the pore velocity \( u \). Therefore, we can either choose to apply the Yao model, recognizing that the filtration equation is based on isolated collectors that do not exist in the packed bed, or use a PV filtration model, recognizing that the Pe number correlation was not developed for the flow conditions arising from flow around spheres in packed beds. To make the filtration model mass balance consistent with the Levich solution, Yao et al. (1971) defined the approach velocity as \( u^* = u \theta \) in the Pe number correlation. However, if the PV filtration equation is used, it makes more sense to use the pore velocity \( u \). Although, each approach has a limiting assumption, it is proposed here that either choice is acceptable as long as the selection of \( u^* \) is consistent with the choice of the characteristic velocity made in deriving the filtration equation.

**Single Collector Efficiencies Based on Happel Model: Yao-Habibian Model**

Discrepancies between the Yao model and observed removal rates led Yao et al. (1971) to propose incorporating a correction factor \( A_t \), derived by Happel (1958) in the collision efficiency term for collisions generated by diffusion. The Happel correction factor \( A_t \), is defined as

\[
A_t = \frac{2(1 - \gamma')}{2 - 3\gamma + 3\gamma^2 - 2\gamma^3}
\]

where \( \gamma = (1 - \theta)^{1/3} \). Including this term transforms (11) to
\[ \eta = 4A^{2/3}N_{pe}^{2/3} + \frac{3}{2}N_{R}^{2/3} + N_{L} \] (13)

which is referred to here as the Yao-Habibian (YH) model. In this approach fluid flow is confined to fit within a concentric spherical space surrounding the collectors. Separate identification of the Yao and YH models is necessary, since researchers citing the Yao model may [e.g., Kinoshita et al. (1993)] or may not [e.g., Harvey and Garabedian (1991)] include the Happel correction term. Once the \( A \) term is included in the collision efficiency equation the choice of the velocity term is no longer arbitrary, since Happel defined it as the superficial velocity in deriving the correction term. The disadvantage of the YH model, from a conceptual perspective, is that the diffusion term is based on flow through a concentric spherical space while the other terms are based on flow around an isolated sphere.

**Clarification of RT Model**

To make all terms in the collision efficiency equation based on flow within a concentric spherical space, Rajagopalan and Tien (1976) developed two equations based on a numerical solution of the differential equation describing particle trajectories to model particle removal by interception and gravitational sedimentation. Their calculations included reductions in collisions due to the resistance of an incompressible fluid when it is pushed out from between two colliding particles, referred to as the lubrication effect, and the effects of London–van der Waals attractive forces. The conceptual advantage of the RT model is that for all filtration mechanisms removal is based on a model that restricts fluid flow to a concentric spherical space surrounding the collectors.

Although the RT model is widely referenced and used, the original publication by Rajagopalan and Tien (1976) and a later review by Tien and Payntakes (1979) contained model equations with hidden constants and typographical errors. According to the original model, the collector efficiency was calculated using

\[ \eta = 4A^{2/3}N_{pe}^{2/3} + [0.72A_{L}^{2/3}N_{R}^{2/3} + 0.0024A_{L}^{2/3}N_{R}^{2/3}] \] (14)

where \( N_{L} \) is an additional term that includes the contributions of particle London–van der Waals attractive forces to particle removal, defined as

\[ N_{L} = \frac{4H}{9\pi \mu d_{s}^{2}U} \] (15)

where \( H \) is the Hamaker constant. The bracketed terms in (14) are the \( \eta \) terms developed by Rajagopalan and Tien using their computer model to predict removal primarily by interception and gravitational sedimentation when \( N_{R} \approx 0.18 \) and \( N_{L} > 0 \). The remaining term for diffusion was assumed valid, based on the YH model, and did not need to be modified for lubrication effects. The fluid velocity used in the solution must be defined as the approach velocity, since this reference velocity was used in developing their model.

One reason the RT model requires clarification is that the "constants" 0.72 and 0.0024 in (14) contain a hidden variable, the column porosity. These constants, 0.72 and 0.0024, are really the products of 3\( \times \frac{\sqrt{2}}{2} \) and two other constants: 2/3 for the first term and 0.00225 for the second term. Rajagopalan and Tien considered a porosity of 0.39 to be typical of packed beds, and therefore presented \( \gamma^{2} \) as a constant equal to 0.72. Subsequent investigators have either cited the incorrect constants (McDowell-Boyer et al. 1986) or have used the corrected constants (with \( \gamma^{2} \) incorporated into the filtration equation) without providing any explanation (Martin et al. 1992).

Eq. (14) also contains an error as indicated in a letter to the editor by Rajagopalan et al. (1982). The first term on the right-hand side of (14) should also be multiplied by \( \gamma^{2} \) in order to correctly reflect the definition of the single collector efficiency that was used in deriving the other terms. The error resulted from not correcting the diffusion term for the flux into the Happel shell as done in the Happel model, whereas in the isolated sphere model the flux is relative to the projected horizontal area of the collector. Incorporating these corrections into \( \eta \) results in

\[ \eta = \gamma^{2}4A^{2/3}N_{pe}^{2/3} + \frac{1}{2}N_{R}^{2/3} + 0.00338A_{L}^{2/3}N_{R}^{2/3} \] (16)

which is correct only when the filtration equation is defined as

\[ \frac{C}{C_o} = \exp \left[ -\frac{3}{2} \frac{(1 - \theta)\gamma^2}{d_c} \alpha \eta L \right] \] (17)

Since all terms on the right-hand side of (16) now contain the \( \gamma^{2} \) term, when (16) and (17) are combined the product of \( \gamma^{2} \) and \( (1 - \theta)^{-3/2} \) produces the term \( (1 - \theta) = \gamma^{2} \). The RT model can equivalently be used with (16) when the collision efficiency is written in the form

\[ \eta = 4A^{2/3}N_{pe}^{2/3} + A_{L}^{2/3}N_{R}^{2/3} + 0.00338A_{L}^{2/3}N_{R}^{2/3} \] (18)

Eq. (17) was not correctly presented in the original work (Rajagopalan and Tien 1976) or corrected in subsequent work (Tien and Payntakes 1979). Correct forms of the RT model have been understood and correctly used, but not previously explained, by others (Martin et al. 1992; Tobaison and O’Melia 1988).

**COMPARISON OF FILTRATION MODELS**

The different predictions of the four filtration models (Yao, PV, YH, and RT) can be seen by comparing particle removal calculated with these models with those reported by Yao et al. (1971, Fig. 6) for completely destabilized latex microspheres in laboratory columns. The filtration equations and collector efficiency equations used for each model were selected to provide a consistent set of assumptions for the mass balance (Table 1). That is, we did not include the Happel correction factor in either the Yao or PV models, since the physical model assumed for the diffusion term (flow restricted to concentric spheres by adjacent collectors) is not the same

<table>
<thead>
<tr>
<th>Model (1)</th>
<th>Filtration equation (2)</th>
<th>Collision efficiency equation (3)</th>
<th>Comments (4)</th>
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</thead>
<tbody>
<tr>
<td>Yao</td>
<td>1</td>
<td>11</td>
<td>Isolated collector; characteristic velocity is approach velocity.</td>
</tr>
<tr>
<td>Pore velocity (PV)</td>
<td>2</td>
<td>11</td>
<td>Collector in packed bed; characteristic velocity is pore velocity.</td>
</tr>
<tr>
<td>Yao-Habibian (YH)</td>
<td>1</td>
<td>13</td>
<td>Same as Yao model, except diffusion term is based on flow in a concentric sphere around collector.</td>
</tr>
<tr>
<td>Rajagopalan and Tien (RT)</td>
<td>17 or 1</td>
<td>16 or 18</td>
<td>All terms based on flow in a concentric sphere; includes lubrication term for all terms except diffusion (lubrication effects are insignificant for collisions by diffusion).</td>
</tr>
</tbody>
</table>

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as assumed for the interception and sedimentation terms (isolated sphere in an infinite fluid).

The PV model predicts greater particle attenuation than the Yao model (Fig. 2), since removal is increased by a factor of $\exp(0.135)$ for particle removal by diffusion, and by a factor of $\exp(0)$ for removal by interception. Therefore, when both the Yao and PV models are applied to the same set of data, $\alpha$ is calculated to be lower using the PV model. Sticking coefficients larger than unity are still considered to be significant, though new to account for the observed removals (Table 2). Using the Yao model, we calculated sticking coefficients from 1.7 to 4.6, compared to only 1.2–3.2 using the PV model and 0.46–4.0 using the YH model. The sticking coefficients calculated using the RT (Fig. 2) model range from 0.46 to 1.1 (Table 2) and are closer to unity than those calculated using the Yao model (for each particle size). Based on these results, and other experience with these models, we recommend that the RT model be used to calculate aerosol removals in packed beds.

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APPENDIX I. REFERENCES


APPENDIX II. NOTATION

The following symbols are used in this paper:

$A = $ cross-sectional area ($L^2$);

$A_i = $ dimensionless Happel correction factor;

$a = $ number of particles that have accumulated in column;

$C = $ effluent particle concentration ($L^{-1}$);

$C_{0i} = $ influent particle concentration ($L^{-1}$);

$c = $ particle concentration in fluid ($L^{-3}$);

$c_i = $ particle concentration in column fluid at point $z$ ($L^{-3}$);

$D = $ column dispersion coefficient ($L^2 T^{-1}$);

$D_{cc} = $ colloid diffusion coefficient ($L^2 T^{-1}$);

$d_i = $ diameter of spherical collector in packed bed ($L$);

$d_{col} = $ colloidal diameter ($L$);

$g = $ gravitational constant ($L T^{-2}$);

$H = $ Hamaker constant, assumed here to be $10^{-13}$ erg (M $L^{-2} T^{-2}$);

$L = $ length of column ($L$);

$N = $ number of collectors in control volume ($V$);

$N_i = $ dimensionless gravitation number, $N_{ci} = U_i/u*$;

$N_{0i} = $ dimensionless number that incorporates London–van der Waals attractive forces, $N_{0i} = 4H/(9\pi u^2)$;

$N_{0i} = $ dimensionless Peclet number, $N_{*i} = u d_i/D_i$;

$N_i = $ dimensionless interception number, $N_{i} = d_i/d*$;

$Q_i = $ rate particles flow toward collector ($T^{-1}$);

$Q_i = $ rate particles strike collector ($T^{-1}$);

$t = $ time ($T$);
\[ U = \text{superficial or approach velocity, } U = u \theta \text{ (L T}^{-1}) \];
\[ U_s = \text{colloid settling velocity (L T}^{-1}) \];
\[ u = \text{interstitial or pore velocity, } u = U/\theta \text{ (L T}^{-1}) \];
\[ u^* = \text{characteristic velocity; either interstitial or pore velocity (L T}^{-1}) \];
\[ V = \text{control volume (}\Delta V\text{) of thickness } \Delta z \text{ and cross-sectional area } A \text{ (L)} \];
\[ z = \text{distance in column (L)} \];
\[ \alpha = \text{sticking coefficient, defined as ratio of rate particles stick to collector to rate they strike collector} \];
\[ \gamma = \text{dimensionless parameter, defined as } \gamma = (1 - \theta)^{1/3} \];
\[ \eta = \text{single collector collision efficiency} \];
\[ \theta = \text{packed bed porosity} \];
\[ \mu = \text{fluid dynamic viscosity (M L}^{-1} \text{T}^{-1}) \];
\[ \rho_f = \text{fluid density (M L}^{-3}) \text{; and} \]
\[ \rho_p = \text{colloid density (M L}^{-3}) \].