Technical University of Denmark

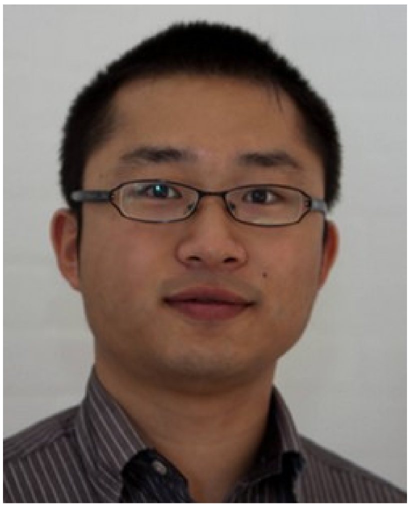
ParPor: Particles in Pores. Stochastic Modeling of Polydisperse Transport

Yuan, Hao

Published in:
DTU Chemical Engineering Graduate School Yearbook 2009

Publication date:
2010

Document Version
Publisher's PDF, also known as Version of record



Hao Yuan

Phone: +45 4525 2960
Fax: +45 4525 2258
E-mail: hy@kt.dtu.dk
WWW: http://www.ivc-sep.kt.dtu.dk/
Supervisors: Alexander Shapiro
Erling Stenby

PhD Study
Started: Oct. 2009
To be completed: Oct. 2012

ParPor: Particles in Pores. Stochastic Modeling of Polydisperse Transport

Abstract

Liquid flow containing particles in the different types of porous media appear in a large variety of practically important industrial and natural processes. The project aims at developing a stochastic model for the deep bed filtration process in which the polydisperse suspension flow in the polydisperse porous media. Instead of the traditional parabolic Advection-Dispersion Equation (ADE) the novel elliptic PDE based on the Continuous Time Random Walk is adopted for the particle size kinetics [1, 2]. The pore kinetics is either described by the stochastic size exclusion mechanism or the incomplete pore plugging model[3, 4]. In the current phase of the project the computation is only performed for the polydisperse suspension flow in monodisperse porous media. The slower transport speed of the peak and larger tail indicates that the elliptic model is more adaptable for anomalous diffusion. Porosity decline of the porous media and convection acceleration of the flow are observed from the modeling results which agree with the general experimental observation.

Introduction

Liquid flow containing particles in the different types of porous media appear in a large variety of practically important industrial and natural processes. A large body of applications has resulted in a large body of research; the researchers from the different areas have scarcely exchanged results and ideas though. The studies may roughly be classified into the two categories: Microscopic, detailed analysis of the particle-pore interactions and of the individual or collective particle behavior on the pore level; and modeling of the particle suspension flows in porous media on the macroscopic level, in the volume larger than REV containing a number of particles and pores. The latter is being focused on in the project.

Macroscopic modeling of the suspension flows in porous media is often based on a hydrodynamic model of the advection-dispersion type, which typically takes the parabolic PDE form (ADE). Particle deposition is modeled similar to “the first order chemical reaction”. Such approach does not account for polydispersity: both particles and pores may be of different sizes and possess different properties, which strongly affects both transport and deposition. Several discrepancies between predicted and observed pictures of filtration were observed in the experiments [5, 6]. These discrepancies are important for practice: for example, porous media lead to separation of the different particles. The particles of the different sizes move with the different microscopic velocities and may be dispersed in the different ways, which leads to the different kind of transport than the classical “diffusion-like” evolution. This may happen even with the particles of the same size (and even with the molecules of a tracer). They may be delayed indefinitely in the pores and then move further. Variability on the pore level leads to dispersion of the particle flight times and to non-conventional transport equations.

The process of suspension flow in porous media is stochastic in nature, and it calls for stochastic modeling. Several stochastic models emerged recently. The continuous-time random walks (CTRW) approach [7, 8]has been applied suspension and tracer flows [6, 9]with effectively monodisperse, but randomly “walking” particles. This approach has managed to explain some (but not all the) experimental results relevant to time dispersion of the particle flights. Based on this theory Pavel and Shapiro developed a novel elliptic model differing from the conventional parabolic ADE [1, 2].

The pore kinetics is either described by the size exclusion mechanism, adsorption, bridging, or other mechanisms which may cause incomplete pore plugging[3, 10]. The porosity decline leads to the convection acceleration of local fluid velocity. This leads to the non-linearity of the elliptic PDE which requires special technique to implement fast computation.

Particle size kinetics

The equation of particle size kinetics should be obtained from a microscopic and stochastic point of view. Following a similar procedure to that in Ref[2], we start with a so-called continuous-time random walker which represents a particle carried by the advection flux from one pore to another, as seen in **Figure 1**.

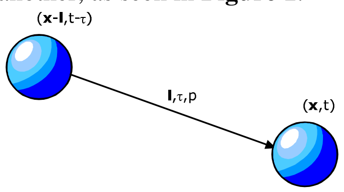


Figure 1: an arbitrary continuous-time random walker's step

As mentioned above the particle may pass through the same pore along different paths. The portion of particles along one path is denoted by $c(\mathbf{l},\tau,r_s,\mathbf{x},t)$, in which the flow direction and the flight time reflect the particle velocity. $c(\mathbf{l},\tau,r_s,\mathbf{x},t)$ is better to be understood as the probability of the condition $(\mathbf{l},\tau,r_s,\mathbf{x},t)$ to happen. p is the probability for the particle to pass the pore under the condition $(\mathbf{l},\tau,r_s,\mathbf{x},t)$, p ranges from 0 to 1.

$$P(\mathbf{l},\tau,p,r_s,\mathbf{x},t)=f(p\,|\,\mathbf{l},\tau,r_s,\mathbf{x},t)c(\mathbf{l},\tau,r_s,\mathbf{x},t)$$

The probability distribution for the walker to appear at (**x,** t) is associated with the PDF for walker to appear at (**x-l,** t-τ) by the convolution law:

$$\begin{aligned}
&\phi(\mathbf{x},t,r_s)C(\mathbf{x},t,r_s)\\
&=pP(\mathbf{l},\tau,p,r_s,\mathbf{x},t)*\left[\phi(\mathbf{x}-\mathbf{l},t-\tau)C(\mathbf{x}-\mathbf{l},t-\tau,r_s)\right]\\
&=\int_0^\infty\int_0^\infty\int_0^1 d^d\mathbf{l}d\tau dp\begin{Bmatrix}pf(p\,|\,\mathbf{l},\tau,r_s,\mathbf{x},t)c(\mathbf{l},\tau,r_s,\mathbf{x},t)\times\\ \left[\phi(\mathbf{x}-\mathbf{l},t-\tau)C(\mathbf{x}-\mathbf{l},t-\tau,r_s)\right]\end{Bmatrix}
\end{aligned}$$

where the superscript 'd' represents the number of dimensions. $C(x,t,r_s)$ is the number of particles of r_s at (x,t). $c(\mathbf{l},\tau,r_s,x,t)$ is the PDF for the particles of r_s randomly walking along the vector **l**. Further reformations of the equation above lead to the following elliptic PDE for one particle size finally:

$$\begin{aligned}
&\partial(\phi C)/\partial t+\mathbf{u}\cdot\nabla(\phi C)\\
&=D_{\mathbf{x}}\nabla^2(\phi C)+D_t\frac{\partial^2(\phi C)}{\partial t^2}+D_{\mathbf{x}t}\frac{\partial(\nabla\phi C)}{\partial t}-\Lambda(\phi C)
\end{aligned}$$

where the detailed coefficients and moments, when time interval is infinitesimal, are:

$$\mathbf{u}(r_s,\mathbf{x},t)=\langle\mathbf{l}\rangle_p/\langle\tau\rangle_p;D_t(r_s,\mathbf{x},t)=\langle\tau^2\rangle_p/2\langle\tau\rangle_p$$

$$D_{\mathbf{x}}(r_s,\mathbf{x},t)=\langle\mathbf{l}^2\rangle_p/2\langle\tau\rangle_p;\quad D_{\mathbf{x}t}(r_s,\mathbf{x},t)=\langle\mathbf{l}\tau\rangle_p/2\langle\tau\rangle_p$$

$$\Lambda(r_s,\mathbf{x},t))=\left(1-P(r_s,\mathbf{x},t)\right)/\langle\tau\rangle_p$$

$$\langle\mathbf{l}\rangle_p=\int_0^\infty\int_0^\infty\int_0^1 d^d\mathbf{l}d\tau dp\{\mathbf{l}pf(\mathbf{l},\tau,p\,|\,r_s,\mathbf{x},t)\};$$

$$\langle\mathbf{l}^2\rangle_p=\int_0^\infty\int_0^\infty\int_0^1 d^d\mathbf{l}d\tau dp\{\mathbf{l}^2pf(\mathbf{l},\tau,p\,|\,r_s,\mathbf{x},t)\};$$

$$\langle\tau\rangle_p=\int_0^\infty\int_0^\infty\int_0^1 d^d\mathbf{l}d\tau dp\{\tau pf(\mathbf{l},\tau,p\,|\,r_s,\mathbf{x},t)\};$$

$$\langle\tau^2\rangle_p=\int_0^\infty\int_0^\infty\int_0^1 d^d\mathbf{l}d\tau dp\{\tau^2pf(\mathbf{l},\tau,p\,|\,r_s,\mathbf{x},t)\};$$

$$\langle\mathbf{l}\tau\rangle_p=\int_0^\infty\int_0^\infty\int_0^1 d^d\mathbf{l}d\tau dp\{\mathbf{l}\tau pf(\mathbf{l},\tau,p\,|\,r_s,\mathbf{x},t)\};$$

The last sink term in represents the retention rate which reflects the capture probability (1-p) on the microscopic level, and this coefficient physically represents the retention probability per unit length of porous media and per unit time. The first coefficient **u** which is the average of step length divided by the average of waiting time is actually the average particle velocity in the pore.

Pore kinetics

The pore structure is changed only when the particles are captured by the pores. To reveal the random process the introduction of a probability for the pore size change is convenient and also necessary for the case of incomplete pore plugging[3]. Let us introduce such a probability ($r_p \rightarrow r_p'$) as the probability of the pore radius changing from r_p to r_p' while capturing a particle of r_s, i.e. when a particle of r_s is captured at **x**,t the pore radius is changed from r_p into r_p', the distribution of r_p is $f(r_p|r_s,\mathbf{x},t)$, the distribution of r_p' is $f(r_p'|r_s,\mathbf{x},t)$, the total probability is:

$$P_d(r_s,\mathbf{x},t,r_p\rightarrow r_p')=P_d(r_s,\mathbf{x},t)f(r_p\,|\,r_s,\mathbf{x},t)f(r_p'\,|\,r_s,\mathbf{x},t);$$

$$P_d(r_s,\mathbf{x},t,r_p\rightarrow r_p')=0:\ r_p\le r_p';$$

$$f(r_p'\,|\,r_s,\mathbf{x},t)=0:\ r_p\le r_p';$$

$$\int_0^\infty P_d(r_s,\mathbf{x},t,r_p\rightarrow r_p')dr_p'=P_d(r_s,\mathbf{x},t)f(r_p\,|\,r_s,\mathbf{x},t);$$

$$\int_0^{r_p} P_d(r_s,\mathbf{x},t,r_p\rightarrow r_p')dr_p'=P_d(r_s,\mathbf{x},t)f(r_p\,|\,r_s,\mathbf{x},t);$$

The second equation above corresponds reflects the fact that the particle will and can only decrease the size of the pore. The resulted integration p_d $(r_s,r_p,\mathbf{x},t)$ the total probability for the particles of r_s being captured by the pores of r_p at (**x**,t). The introduction of such a probability is nontrivial in the following sense. The pore kinetics is described on the premise of the pore of r_p capturing a particle of r_s; both of the pore and particle shape parameters are known. Nonetheless the pore size change is still random. This can be illustrated by **Figure 2**, in which the resulted pore shape parameter is random due to the random capture process.

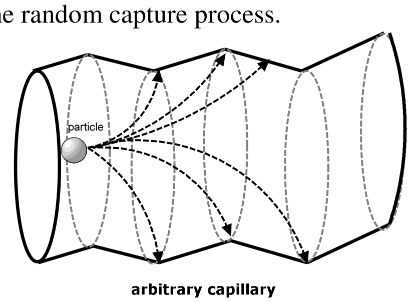


Figure 2: the random capture process of a particle smaller than the pore

Here the governing equations for the pore evolution are obtained following a similar procedure as in Ref[3]. The change of the pore distribution of r_p is revealed by the increasing term and a decreasing term. Larger pores than those of r_p capturing particles may increase the number the pores of r_p. Pores of r_p capturing particles leads to decreasing the number of pores of r_p.

$$H(\mathbf{x},t,r_s,r_p)-H(\mathbf{x},t-\tau,r_s,r_p)=I(\mathbf{x},t,r_s,r_p)-D(\mathbf{x},t,r_s,r_p)$$

where I represent the increase rate and D represents the decrease rate of the number of pores of r_p during the time τ. Since the particle capture does not influence the pore length, the pore distribution adopted here does not depend on the pore length. Define the probability to have 1-p for a particle to be captured simultaneously with the setting (l,τ,r_s,p,x,t):

$$P_d(\mathbf{l},\tau,p,r_s,\mathbf{x},t)=P_d(r_s,\mathbf{x},t)f(\mathbf{l},\tau,p\,|\,r_s,\mathbf{x},t)$$

where $P_d(r_s,\mathbf{x},t)$ is total probability for a particle of r_s being captured, this is defined in the same fashion as regarding the particle passing the pore. The probability for a particle to be captured with the setting (l,τ,r_s,p,x,t):

$$(1-p)P_d(\mathbf{l},\tau,p,r_s,\mathbf{x},t)=\left(1-pf(p\,|\,\mathbf{l},\tau,r_s,\mathbf{x},t)\right)c(\mathbf{l},\tau,r_s,\mathbf{x},t)$$

According to definition of microscopic p_d the probability for the particle of r_s being captured, with the particle flight as (l,τ,p) and the pore of r_p to be changed into r_p':

$$P_d(\mathbf{l},\tau,p,r_s,\mathbf{x},t,r_p\to r_p^{'})$$
$$=P_d(\mathbf{l},\tau,p,r_s,\mathbf{x},t)f\left(r_p\,|\,\mathbf{l},\tau,p,r_s,\mathbf{x},t\right)f\left(r_p^{'}\,|\,\mathbf{l},\tau,p,r_s,\mathbf{x},t\right)$$

With the obtained probability above the decreasing term can be formulated as:

$$D(\mathbf{x},\mathrm{t},r_s,\mathrm{r_p})$$
$$=\int_0^1\int_0^{r_p}dpdr_p^{'}\begin{Bmatrix}(1-p)P_d(\mathbf{l},\tau,p,r_s,\mathbf{x},t,r_p\to r_p^{'})*\\ \left[\phi(\mathbf{x}-\mathbf{l},t-\tau)C(\mathbf{x}-\mathbf{l},t-\tau,r_s)\right]\end{Bmatrix}$$
$$=\int_0^\infty\int_0^\infty\int_0^1\int_0^{r_p}d\mathbf{l}d\tau dpdr_p^{'}$$
$$\begin{Bmatrix}(1-p)P_d(\mathbf{l},\tau,p,r_s,\mathbf{x},t)f\left(r_p\,|\,\mathbf{l},\tau,p,r_s,\mathbf{x},t\right)\times\\ f\left(r_p^{'}\,|\,\mathbf{l},\tau,p,r_s,\mathbf{x},t\right)\left[\phi(\mathbf{x}-\mathbf{l},t-\tau)C(\mathbf{x}-\mathbf{l},t-\tau,r_s)\right]\end{Bmatrix}$$

According to the property of p_d the integral for r_p' can be reduced to:

$$D(\mathbf{x},\mathrm{t},r_s,\mathrm{r_p})=\int_0^\infty\int_0^\infty\int_0^1 d\mathbf{l}d\tau dp$$
$$\begin{Bmatrix}(1-p)P_d(\mathbf{l},\tau,p,r_s,\mathbf{x},t)f(r_p\,|\,\mathbf{l},\tau,p,r_s,\mathbf{x},t)\times\\ \left[\phi(\mathbf{x}-\mathbf{l},t-\tau)C(\mathbf{x}-\mathbf{l},t-\tau,r_s)\right]\end{Bmatrix}$$

Taylor expansion of the inside of the integral leads to the total equation for the pore kinetics:

$$D(\mathbf{x},\mathrm{t},r_s,\mathrm{r_p})=\int_0^\infty\int_0^\infty\int_0^1 d\mathbf{l}d\tau dp$$
$$\begin{Bmatrix}(1-p)P_d(\mathbf{l},\tau,p,r_s,\mathbf{x},t)f(r_p\,|\,\mathbf{l},\tau,p,r_s,\mathbf{x},t)\times\\ \begin{pmatrix}\phi(\mathbf{x},t)C(\mathbf{x},t,r_s)-\mathbf{l}\dfrac{\partial(\phi C)}{\partial\mathbf{x}}-\tau\dfrac{\partial(\phi C)}{\partial t}\\ -\mathbf{l}^2\dfrac{\partial^2(\phi C)}{\partial\mathbf{x}^2}-\tau^2\dfrac{\partial^2(\phi C)}{\partial t^2}-\mathbf{l}\tau\dfrac{\partial^2\phi C}{\partial t\partial\mathbf{x}}\end{pmatrix}\end{Bmatrix}$$

Further reformations lead to the following elliptic PDE form inside the integral:

$$\frac{\partial\mathrm{H}(\mathbf{x},\mathrm{t},\mathrm{r_s},\mathrm{r_p})}{\partial t}=$$
$$P_d(r_s,\mathbf{x},t)f(r_p\,|\,r_s,\mathbf{x},t)\times\left[1-\int_{r_p}^\infty dr_p^{'}f\left(r_p^{'}\,|\,r_s,\mathbf{x},t\right)\right]$$
$$\begin{Bmatrix}\dfrac{\partial(\phi C)}{\partial t}+\mathbf{u}_d(r_s,\mathbf{x},t)\dfrac{\partial(\phi C)}{\partial\mathbf{x}}+D_{\mathbf{x}d}(r_s,\mathbf{x},t)\dfrac{\partial^2(\phi C)}{\partial\mathbf{x}^2}\\ +D_{td}(r_s,\mathbf{x},t)\dfrac{\partial^2(\phi C)}{\partial t^2}+D_{\mathbf{x}td}(r_s,\mathbf{x},t)\dfrac{\partial^2\phi C}{\partial t\partial\mathbf{x}}\end{Bmatrix}$$

where the coefficients with the subscript 'd' possess almost the same definitions as in the particle kinetics, only the probability for the moments calculation is p_d.

CFD implementation

The numerical solution to this non-linear problem is non-trivial. The present computation is confined to the mechanism of size exclusion, in which the increasing term I in the equation above disappear (one particle remains, one pore dies). Setting the constant flow the fluid is accelerated due to convection. We adopt the matrix form of the elliptic PDE for the particle kinetics, where the four boundary conditions are set as: inject suspension for one fifth of the total injection time then inject water to 'wash away' the particles, so that at the end of time the suspension concentration is zero. After solving once the concentration profile we solve the equations of porosity evolution and the velocity profile with convection acceleration. The iteration with this pattern of calculation continues until converge.

Results

The behavior of the elliptic PDE for the particle kinetics is shown in Figure 3. It can be observed that the velocity of the peak is slower and the tail at the outlet is larger in the elliptic model than those in the parabolic ADE.

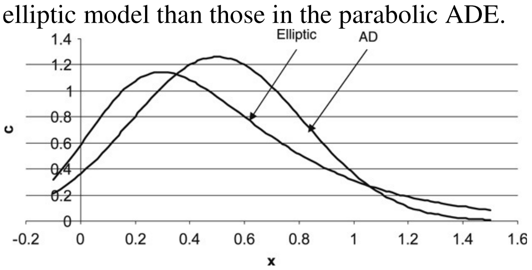


Figure 3: difference between the elliptic model and the parabolic ADE[2]

The concentration profile for the particles of a certain size can be found in Figure 4, in which at the end of injection time all particles are washed away. For particles of n sizes there are n similar profiles like this. The porosity profile in Figure 5 shows that the porosity decline is most dramatic at the inlet. The velocity profile shows that the fluid is accelerated due to convection as in Figure 6. The deposition profile shows that the deposition accumulates mostly at the inlet as seen in Figure 7. This corresponds to the porosity decline profile and the velocity profile.

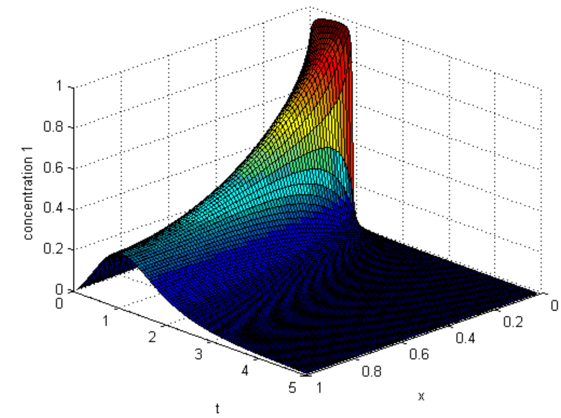


Figure 4: suspension concentration profile

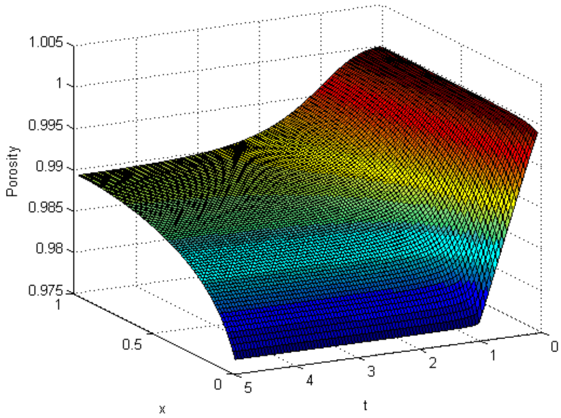


Figure 5: porosity decline profile

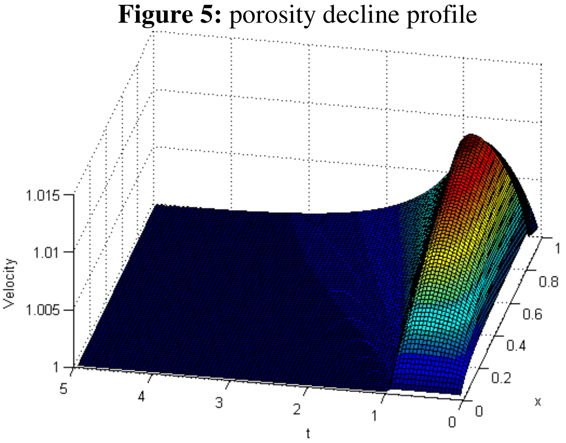


Figure 6: fluid velocity profile

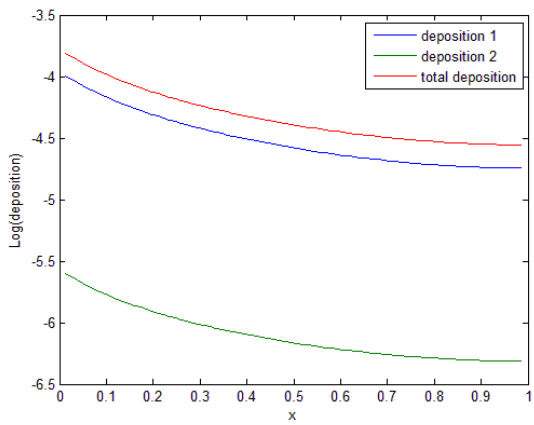


Figure 7: deposition accumulation profile

References

1. Shapiro, A.A., *Elliptic equation for random walks. Application to transport in microporous media.* Physica A: Statistical Mechanics and its Applications, 2007. **375**(1): p. 81-96.
2. Shapiro, A.A. and P.G. Bedrikovetsky, *Elliptic random-walk equation for suspension and tracer transport in porous media.* Physica A: Statistical Mechanics and its Applications, 2008. **387**(24): p. 5963-5978.
3. Shapiro, A., et al., *A stochastic model for filtration of particulate suspensions with incomplete pore plugging.* Transport in Porous Media, 2007. **67**(1): p. 135-164.
4. Santos, A. and P. Bedrikovetsky, *Size exclusion during particle suspension transport in porous media: stochastic and averaged equations.* Computational and Applied Mathematics, 2004. **23**(2-3): p. 259-284.
5. Tufenkji, N. and M. Elimelech, *Breakdown of Colloid Filtration Theory: Role of the Secondary Energy Minimum and Surface Charge Heterogeneities.* Langmuir, 2005. **21**(3): p. 841-852.
6. Tufenkji, N., J.A. Redman, and M. Elimelech, *Interpreting Deposition Patterns of Microbial Particles in Laboratory-Scale Column Experiments.* Environmental Science & Technology, 2003. **37**(3): p. 616-623.
7. Metzler, R. and J. Klafter, *The random walk's guide to anomalous diffusion: a fractional dynamics approach.* Physics Reports, 2000. **339**(1): p. 1-77.
8. Cortis, A. and B. Berkowitz, *Anomalous Transport in "Classical" Soil and Sand Columns.* Soil Sci Soc Am J, 2004. **68**(5): p. 1539-1548.
9. Barkai, E., R. Metzler, and J. Klafter, *From continuous time random walks to the fractional Fokker-Planck equation.* Physical Review E, 2000. **61**(1): p. 132.
10. Herzig, J.P., D.M. Leclerc, and P.L. Goff, *Flow of Suspensions through Porous Media-Application to Deep Filtration.* Industrial & Engineering Chemistry, 1970. **62**(5): p. 8-35.