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Extension of the Feller-Fokker-Planck equation to two and three dimensions for modeling solute transport in fractal porous media

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Abstract. Following an earlier development of a Fokker-Planck equation (FP) for modeling fractal-scale-dependent transport of solutes in one-dimensional subsurface flow of heterogeneous porous media, this technical note extends the FP to three dimensions, and presents a two-dimensional (2-D) FP by reducing the 3-D FP with the aid of the Dupuit approximation. The 2-D FP is derived by including two fractal dispersivities in the convective-dispersive equation leading to a generalized Feller-Fokker-Planck equation (GFFP) featuring both the generalized Feller equation (GF) and FP. Similarity solutions of the 2-D GFP with two linear-scale-dependent dispersivities are presented which can be used as a kernel in the convolution integral to yield an output on a real timescale, and the input function can be derived by a procedure known as the inverse problem with the aid of a Laplace transform.

1. Generalization of the Feller-Fokker-Planck Transport Equation for Subsurface Flow in Physically Heterogeneous Media

In the previous presentation [*Su*, 1995] a scale-dependent fractal dispersivity was introduced in the convective-dispersive equation to yield a one-dimensional Fokker-Planck equation (FP). The present paper extends the procedures to two and three dimensions to generalize the FP.

The governing equation for the movement of a solute present in subsurface flow in a porous medium is [*Javandel et al.*, 1984]

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial c}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(v_i c) - \frac{S}{\phi}Q + \sum_{k=1}^{N} R_k \tag{1}$$

$$v_i = -\frac{k_{ij}}{\phi}\frac{\partial h}{\partial x_j} \tag{2}$$

where

- c solute concentration;
- D_{ij} hydrodynamic dispersion coefficient tensor;
- v_i interstitial velocity in the direction x_i;
- Q volumetric flow rate per unit volume of the source/sink;
- S solute concentration of species in the source/sink fluid;
- R_k rate of production in reaction (adsorption) k of N reactions;
- k_{ij} hydraulic conductivity tensor;
- h hydraulic head;
- x_i Cartesian coordinate;
- ϕ effective porosity;
- t time;
- i, j are counters of coordinates ($i, j = 1, 2, 3$).

For the transport of solutes in subsurface flows in a heterogeneous porous medium in three dimensions with coordinates aligned along the principal axes, (1) can be expanded as

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D_L\frac{\partial c}{\partial x}\right) - \frac{\partial}{\partial x}(uc) + \frac{\partial}{\partial y}\left(D_T\frac{\partial c}{\partial y}\right) - \frac{\partial}{\partial y}(vc) + \frac{\partial}{\partial z}\left(D_v\frac{\partial c}{\partial z}\right) - \frac{\partial}{\partial z}(wc) - \frac{S}{\phi}Q + \sum_{k=1}^{N} R_k \tag{3}$$

where D_L, D_T, and D_v are the longitudinal, horizontal transverse, and vertical transverse hydrodynamic dispersion coefficients, respectively, and v_L, v_T, and v_v are the interstitial velocities in the longitudinal, horizontal transverse, and vertical transverse directions, respectively.

Extensive studies since *Taylor*'s [1953] initiation show that the relationship between D_i and v_i can be represented by an expression of the form

$$D_L = \alpha_L v_L^n \tag{4}$$

and for the two transverse dispersion coefficients, we have

$$D_T = \alpha_T v_T^p \tag{5}$$

$$D_v = \alpha_v v_v^q \tag{6}$$

where α_L, α_T and α_v are the longitudinal, horizontal transverse, and vertical dispersivities, respectively, and n, p, and q are exponents.

Equations (4), (5), and (6) can be modified by using *Wheatcraft and Tyler*'s [1988] fractal model, which is of the form

$$\alpha_L = \tfrac{1}{2}\sigma^2 x^{(2d-1)} \tag{7}$$

where σ^2 is the variance of cutoff limit ε_c, d is the fractal dimension in one dimension, and x is the scale.

If one simplifies the parameters, (7) can be cast into the form

$$\alpha_L = \varepsilon x^m \tag{8}$$

where

$$\varepsilon = \tfrac{1}{2}\sigma^2 \qquad m = 2d - 1$$

Wheatcraft and Tyler [1988, p. 574] show that $d = 1.0865$, i.e., $m \approx 1.0$, and *Tyler and Wheatcraft* [1992, equation (8)] show that $1 < d > 2$.

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Equation (8) can be extended to three dimensions, namely

$$\alpha_L = \varepsilon_L x^f \tag{9}$$

$$\alpha_T = \varepsilon_T y^g \tag{10}$$

$$\alpha_v = \varepsilon_v z^w \tag{11}$$

where ε_L, ε_T, ε_v, f, g, and w are parameters similar in meaning to those in (8).

It should be made clear that the dimension concerning the extension of (8) to three dimensions is the Euclidean dimension and not the fractal dimension, since the fractal structure of the porous medium itself exhibits a multifractal nature [*Korvin*, 1992]. This is comparable to the "flow in a system consisting of fractal object (fracture network) embedded in a Euclidean object (matrix)" [*Chang and Yortsos*, 1990, p. 31], or flow and transport in a fractal medium in a Eulidean space.

Combining (2) with (4)–(6) and (9)–(11) gives

$$D_L = \varepsilon_L x^f \left(-\frac{k(x,y,z)}{\phi} \frac{\partial h}{\partial x} \right)^n \tag{12}$$

$$D_T = \varepsilon_T y^g \left(-\frac{k(x,y,z)}{\phi} \frac{\partial h}{\partial y} \right)^p \tag{13}$$

$$D_v = \varepsilon_v z^w \left(-\frac{k(x,y,z)}{\phi} \frac{\partial h}{\partial z} \right)^q \tag{14}$$

In order to incorporate (12), (13), and (14) into (3), the formulation would be simplified if the hydraulic gradients of an aquifer in a three-dimensional space is represented by the gradients of the phreatic surface in three dimensions based on the Dupuit assumption [*Bear*, 1972, pp. 361–364], i.e.,

$$s_L = -\partial h / \partial x \tag{15}$$

$$s_T = -\partial h / \partial y \tag{16}$$

$$s_v = 0 \tag{17}$$

where s_L, s_T, and s_v are the gradients of the phreatic surface in the x, y, and z directions.

Combining (12)–(17) gives

$$D_L = \varepsilon_L x^f \left(\frac{\bar{K} s_L}{\phi} \right)^n \tag{18}$$

$$D_T = \varepsilon_T y^g \left(\frac{\bar{K} s_T}{\phi} \right)^p \tag{19}$$

where $\bar{K}$ is the head-weighted hydraulic conductivity [*Bear*, 1972, p. 376; *Mariño and Luthin*, 1982, p. 142] given by

$$\bar{K} = \frac{1}{h} \int_0^h k_{(x,y,z)} \, dz \tag{20}$$

Since Dupuit theory applies to the essentially horizontal flow that is equivalent to the case that h deviates only a small amount from a mean depth H, the h in (20) can be replaced by H [*Werner*, 1957; *Mariño and Luthin*, 1982; *Su*, 1995]. Therefore the head-weighted mean hydraulic conductivity is now written

$$\bar{K} = \frac{1}{H} \int_0^H k_{(x,y,z)} \, dz \tag{21}$$

Substituting (15)–(21) in (3) reduces the three-dimensional problem of (3) to

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left[\varepsilon_L x^f \left(\frac{\bar{K}}{\phi} s_L \right)^n \frac{\partial c}{\partial x} \right] - \left(\frac{\bar{K}}{\phi} s_L \right) \frac{\partial c}{\partial x} + \frac{\partial}{\partial y} \left[\varepsilon_T y^g \left(\frac{\bar{K}}{\phi} s_T \right)^p \frac{\partial c}{\partial y} \right] - \left(\frac{\bar{K}}{\phi} s_T \right) \frac{\partial c}{\partial y} - \frac{s}{\phi} Q + \sum_{k=1}^{N} R_k \tag{22}$$

which is the reduced two-dimensional FP, and its solutions are given in the following section.

2. Solutions of (22)

2.1. Similarity Solutions

In (21) and (22) the averaged $\bar{K}$ is a single value. In this case, (22) can be written in the following form with two linear-scale dependent dispersivities, i.e., $f = 1$ and $g = 1$ as demonstrated earlier [*Su*, 1995]:

$$\frac{\partial c}{\partial t} = \frac{\partial^2}{\partial x^2} [A(x)c] - B \frac{\partial c}{\partial x} + \frac{\partial^2}{\partial y^2} [C(y)c] - D \frac{\partial c}{\partial y} - \frac{s}{\phi} Q + \sum_{k=1}^{N} R_k \tag{23}$$

where

$$A(x) = \varepsilon_L x \left(\frac{\bar{K} s_L}{\phi} \right)^n \tag{24}$$

$$B = \varepsilon_L \left(\frac{\bar{K} s_L}{\phi} \right)^n + \frac{\bar{K} s_L}{\phi} \tag{25}$$

$$C(y) = \varepsilon_T y \left(\frac{\bar{K} s_T}{\phi} \right)^p \tag{26}$$

$$D = \varepsilon_T \left(\frac{\bar{K} s_T}{\phi} \right)^n + \frac{\bar{K} s_T}{\phi} \tag{27}$$

The reaction source/sink term in (23) is usually expressed in different forms of isotherms or reactions [*Bird et al.*, 1960; *Javandel et al.*, 1984; *Bear and Buchlin*, 1991]:

$$\sum_{k=1}^{N} R_k = -\frac{\rho}{\phi} \frac{\partial \varsigma}{\partial t} \tag{28}$$

$$\varsigma = \kappa c^\omega \tag{29}$$

where ς is the concentration of species adsorbed on the solid, ρ is the bulk density, and κ and ω are the reaction time parameter and the order of reaction, respectively.

Equations (28) and (29) can be combined to yield

$$\sum_{k=1}^{N} R_k = -\left(\frac{\rho}{\phi} \kappa \omega c^{\omega - 1} \right) \frac{\partial c}{\partial t} \tag{30}$$

Inserting (30) into (23) and rearranging yields

$$\frac{\partial c}{\partial t} R_{t(c)} = \frac{\partial^2}{\partial x^2} [A(x)c] - B \frac{\partial c}{\partial x} + \frac{\partial^2}{\partial y^2} [C(y)c] - D \frac{\partial c}{\partial y} - \frac{s}{\phi} Q \tag{31}$$

where

$$R_{t(c)} = 1 + \left(\frac{\rho}{\phi}\kappa\omega c^{\omega-1}\right) \tag{32}$$

is the retardation equation, and is now concentration-dependent.

For a linear relationship between c and ς, (32) is reduced to

$$R_t = 1 + (\rho\kappa/\phi) \tag{33}$$

which is now a constant, with κ being assigned a different name such as the partition coefficient, κ_p.

For $f = 1.0$ and $g = 1.0$ in (31) and $\omega = 1$ in (32), equation (31) is essentially the form of

$$\frac{\partial c}{\partial t}R_t = \frac{\partial^2}{\partial x^2}[A(x)c] - B\frac{\partial c}{\partial x} + \frac{\partial^2}{\partial y^2}[C(y)c] - D\frac{\partial c}{\partial y} - \frac{s}{\phi}Q \tag{34}$$

where $A_{(x)}$, B, $C_{(y)}$, and D are given by (24), (25), (26), and (27), respectively.

With a Dirac delta function input to (34) [*Hill and Dewynne*, 1987, p. 28],

$$Q_{(x,y,0)} = \frac{M_0}{\phi}\delta(x)\delta(y) \tag{35}$$

$$c_{(x,y,t)} \to 0 \qquad \text{as} \quad t \to \infty \tag{36}$$

where $Q_{(x,y,0)}$ is the mass injection rate; and M_0 is the mass of solute being released at the origin at time zero. The similarity solution of Eq. (34) is

$$c_0(x, y, t) = \frac{x^{\gamma_{Lr}}y^{\gamma_{Tr}}}{\Gamma[\gamma_{Lr}+1]\Gamma[\gamma_{Tr}+1][\alpha_{Lr}t]^{\gamma_{Lr}+1}[\alpha_{Tr}t]^{\gamma_{Tr}+1}} \cdot \exp\left[-\left(\frac{x}{\alpha_{Lr}t}\right) - \left(\frac{y}{\alpha_{Tr}t}\right)\right] \tag{37}$$

where $\Gamma[\gamma_{Lr} + 1]$ and $\Gamma[\gamma_{Tr} + 1]$ are the Gamma functions of $[\gamma_{Lr} + 1]$ and $[\gamma_{Tr} + 1]$, respectively;

$$\alpha_{Lr} = \frac{\varepsilon_L}{R_t}\left(\frac{\bar{K}s_L}{\phi}\right)^n \tag{38}$$

$$\gamma_{Lr} = \frac{1}{\varepsilon_L R_t}\left(\frac{\bar{K}s_L}{\phi}\right)^{1-n} \tag{39}$$

$$\alpha_{Tr} = \frac{\varepsilon_T}{R_t}\left(\frac{\bar{K}s_T}{\phi}\right)^p \tag{40}$$

$$\gamma_{Tr} = \frac{1}{\varepsilon_T R_t}\left(\frac{\bar{K}s_T}{\phi}\right)^{1-p} \tag{41}$$

which are derived following the procedures shown by *Su* [1995].

For conservative solutes, $R_t = 1$. Then (37) reduces a similarity solution for the transport of conservative solutes.

2.2. Solutions Subject to Arbitrary Inputs and the Inverse Problem

The similarity solution corresponds to an instantaneous input at the origin at zero time. For an arbitrary time-dependent input at the boundary of $x = 0$, the convolution integral of the similarity solution gives the actual distribution of the solute concentration, $C_{(x,y,t)}$. In order to derive the input function, Laplace transform and numerical inversion techniques can be used, which is beyond the scope of this paper.

3. Concluding Remarks

Following a previous paper [*Su*, 1995] presenting a scale-dependent, one-dimensional, convective-dispersive equation of transport in subsurface flow known as the second diffusion equation or the Fokker-Planck equation, this note generalizes this approach by presenting a scale-dependent, two-dimensional, convective-dispersive equation of transport in subsurface flow in heterogeneous porous media, which is designated as generalized Feller-Fokker-Planck equation (GFFP) since it incorporates the features of both the generalized Feller equation and the Fokker-Planck equation. Similarity solutions of the 2-D GFFP are presented. Since the coefficients of FP are essentially functions of the transported materials and the media, investigations of characteristics of these coefficients in this area are very important.

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