

Derivation of the Convective Dispersion Equation with Adsorption by Markov Random Ways

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(Received 9 March 2009)

The convective dispersion equation with adsorption is derived on the basis of the Chapman–Kolmogoroff equation which expresses the statistical properties of the Markov transition probability. The acquired equation has the same expression as the one derived on the basis of the combination of both the mass balance equation and the particles retention kinetics equation. The probability variables that describe the random movement of solute particles have a definite physical significance associated with the parameters in the convective dispersion equation. The derivation confirms the validity of the Markov process to describe the particles movement in the process of convective dispersion.

PACS: 47.56.+r, 47.27.eb

In the process of groundwater transportation, the combined effects of the molecular diffusion and mechanical dispersion of the solute particles make the front edge of the displacing fluid not a transitional region with a uniform or a sudden change.^[1–5] Many physical and chemical reactions that occur in this area have a great influence on both the overall transportation of the solute and its concentration distribution inside porous media, and understanding these laws of solute transportation and distribution is useful for controlling of groundwater contamination^[6,7] in environment protection and the enhancement of oil displacement efficiency by chemical agents.^[2,8,9] Many studies in this area have been performed either at laboratories or by mathematical modeling. Via a laboratory method, Fick obtained the first Fick's law that describes stable status diffusion, and he then deduced the second Fick's law for describing unstable diffusion. Aiming at the model provided by Iwasa^[10], that did not consider the hydrodynamic dispersion, Altoé *et al.*^[11] took the dispersive effect into consideration in the particles retention kinetics equation and constructed a complete deep filtration model on the basis of the mass balance equation of the suspension. Using the method of infinitesimal volume, Ge *et al.*^[12] derived different differential forms of the convective dispersion equations for the ideal condition and the actual conditions including the viscosity difference or the adsorption. Recently, new methods like fractal^[13–15] and fractional differentiation^[16–19] were proposed to construct dispersive models of solute transportation. At the same time, the statistical nature of the behavior has been observed in the convective dispersion of solute particles, as the concentration distribution at the front edge of dispersion is the cumulative result of the random walk of a large number of particles. After analyzing a great number of experimental data statis-

tically, Wu *et al.*^[20] investigated the randomness of parameters in the dispersion equation. The molecular dynamics simulation used to model the characteristic of motion of solute particles has solid foundations in probability theory.^[21,22] Many authors also obtained the probability solution to the convective dispersion equation.^[11,12,23] However, there is no report of the complete derivation of the convective dispersion equation based on the theory of probability statistics so as to provide direct support to the randomness of the convective dispersion equation. In this Letter, the convective dispersion equation with adsorption is derived according to the Chapman–Kolmogoroff equation which is used to describe the transition probability of the Markov process.

The distinct characteristics of the Markov process lie in the memorylessness of the former behaviors, and its transition probability is expressed by the Chapman–Kolmogoroff equation^[24]

$$p(x_3, t_3|x_1, t_1) = \int p(x_3, t_3|x_2, t_2) \cdot p(x_2, t_2|x_1, t_1) dx_2. \quad (1)$$

For a Markov process, in any case, if $\varepsilon > 0$ and the following expression remains correct for any z , t and Δt , the samples' route is a continuous function of their probability all the way up to 1.

$$\lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int_{|x-z|>\varepsilon} p(x, t + \Delta t|z, t) dx = 0. \quad (2)$$

The Chapman–Kolmogoroff equation can be transformed to a differential form under the proper presumed condition which is closely related to the continuous quality of the process. According to Eq. (2) of the continuity condition, effort is made to divide the differentiation condition into several parts, one part

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corresponds to the continuous movement of some typical particles, and the others correspond to the discontinuous movement.

For $\varepsilon > 0$, in any case, the following expressions must be correct:

$$(i) \quad \lim_{\Delta t \rightarrow 0} p(x, t + \Delta t | z, t) / \Delta t = W(x | z, t). \quad (3)$$

If $|x - z| > \varepsilon$ and Eq. (3) is correct for all of x , z and t , then

$$(ii) \quad \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int_{|x-z| < \varepsilon} (x_i - z_i) p(x, t + \Delta t | z, t) dx = A_i(z, t) + O(\varepsilon), \quad (4)$$

$$(iii) \quad \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int_{|x-z| < \varepsilon} (x_i - z_i)(x_j - z_j) \cdot p(x, t + \Delta t | z, t) dx = B_{ij}(z, t) + O(\varepsilon). \quad (5)$$

Equations (4) and (5) are correct for all z , ε and t .

According to Eq. (2), the continuity condition, if $W(x | z, t) = 0$ for all $x \neq z$, there is only a continuous route for this process. Then, this function necessarily describes a discontinuous movement in a certain way, while the variables A_i and B_{ij} are inevitably associated with the continuous movement.

In the sum of the above continuity condition and presumed conditions, the differential form of the Chapman–Kolmogoroff equation was derived as^[24]

$$\begin{aligned} \partial_t p(z, t | y, s) = & - \sum_i \frac{\partial}{\partial z_i} A_i(z, t) p(z, t | y, s) \\ & + \frac{1}{2} \sum_{i,j} \frac{\partial^2}{\partial z_i \partial z_j} B_{ij}(z, t) p(z, t | y, s) \\ & + \int [W(z | x, t) p(x, t | y, s) \\ & - W(x | z, t) p(z, t | y, s)] dx. \end{aligned} \quad (6)$$

In a circular physical sand model initially saturated with crude oil, at time $t = 0$ a solution with a certain concentration of a chemical agent is injected from the inlet. Thus at the beginning ($t = 0$) the interface between the saturated fluid and the flooded liquid locates at the site $x = 0$. The concentration of the displacing solution on the left side of the interface follows the equation $c = c_1$ while in the core that locates at the right of the interface the concentrations of the displaced liquid follow the equation $c = 0$, see Fig. 1.

At the initial time $t = 0$, the substance in solution is carried out from the inlet towards the outlet inside the core. Afterwards, the locations of solute particles at any time $t > 0$ form a one-dimensional random vector $(\xi_t, t \geq 0)$. When t changes in the parameters set $T \in [0, \infty]$, $\{\xi_t, t \geq 0\}$ denotes a random process.

If $\xi_s = y$ at time $t = s$ is known, the distribution $\xi_t (t > s)$ is independent of the values before time s because of the randomness of both the pores, channels

and the particles' movement. According to the definition of the Markov process, $\{\xi_t, t \geq 0\}$ is a Markov process. Its transition probability distribution function can be expressed as $F(x, t; y, s) = P(\xi_t \leq x | \xi_s = y)$. If the probability density is denoted by $f(y, t; x, s)$, there is an expression $f(x, t; y, s) = \partial F(x, t; y, s) / \partial x$. Because there exists the phenomenon of the solute particles in the porous media, it can be presumed that $f(x, t; y, s)$ complies with the following three conditions for any number of ε and Δt if $\varepsilon > 0$ and $\Delta t > 0$.

$$\lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int_{|x-y| > \varepsilon} f(x, t + \Delta t; y, t) dx = 0, \quad (7)$$

$$\lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int_{|x-y| < \varepsilon} (x - y) \cdot f(x, t + \Delta t; y, t) dx = A(y, t), \quad (8)$$

$$\lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int_{|x-y| < \varepsilon} (x - y)^2 \cdot f(x, t + \Delta t; y, t) dx = B(y, t). \quad (9)$$

Equation (7) shows that the probability that the solute particle moves away from the space interval (y, x) within Δt since the initial time t at the beginning point y is an infinitesimal of higher order than Δt . It explains that solute particles cannot cover a big distance within a short time in the pore-channels. That is, the particle moves continuously. Under condition (7), the variable $A(y, t)$ in Eq. (8) has the physical meaning of the average speed within Δt for particles starting at time t by point y , and $B(y, t)$ is related to the average sweep area. Thus $\{\xi_t, t \geq 0\}$ is a convective dispersion process.

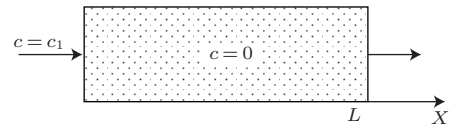


Fig. 1. Flow model in porous medium.

Then the differential Chapman–Kolmogoroff equation can be reduced to the Fokker–Planck equation, of which the one-dimensional expression is shown as follows:

$$\begin{aligned} \frac{\partial f(x, t | y, s)}{\partial t} = & - \frac{\partial}{\partial x} [A(y, t) f(x, t | y, s)] \\ & + \frac{1}{2} \frac{\partial^2}{\partial x^2} [B(y, t) f(x, t | y, s)]. \end{aligned} \quad (10)$$

It corresponds to the mathematical diffusion process where $A(y, t)$ is a drift vector and $B(y, t)$ is a diffusion matrix. If $W(z | x, t) = 0$, then the requirement for the continuity route can be satisfied. Thus the Fokker–Planck equation describes a process with the continuity route $X(t)$.

In Eq. (10), the detailed expressions for $A(y, t)$ and $B(y, t)$ and their partial differential forms are deduced

in the following. Under condition (7), Eq. (8) can be transformed to

$$\lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} E[\xi_{t+\Delta t} - \xi_t | \xi_t = y] = A(y, t), \quad (11)$$

where $A(y, t)$ is the quotient of the average random displacement to the time difference and $A(y, t)$ should mean the average fluid speed of the solute particles in the porous media that is denoted by v .

$$A(y, t) = v. \quad (12)$$

Under condition (7), Eq. (9) can be transformed to

$$\lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} E[(\xi_{t+\Delta t} - \xi_t)^2 | \xi_t = y] = B(y, t). \quad (13)$$

According to Ref. [25], the dispersion coefficient D can be defined by the quotient of the variance σ to time as

$$D = \sigma/2t, \quad (14)$$

by the definition of variance

$$\lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} E[(\xi_{t+\Delta t} - \xi_t)^2 | \xi_t = y] = B(y, t) = 2D. \quad (15)$$

Now the differential form of $A(y, t)$ can be derived from Eq. (8) as

$$\frac{\partial A(y, t)}{\partial x} = \lim_{\Delta t \rightarrow 0} \frac{(x-y)f(x, t+\Delta t; y, t)}{\Delta t}. \quad (16)$$

Equation (16) indicates that some particles travel from point y at time t to the point x by convective dispersion with a probability density $f(x, t+\Delta t; y, t)$ and a speed $(x-y)/\Delta t$. If these particles are captured at a statistical average speed v and with a constant probability density λ in the fluid flowing direction, then

$$\frac{\partial A(y, t)}{\partial x} = \lim_{\Delta t \rightarrow 0} \frac{(x-y)f(x, t+\Delta t; y, t)}{\Delta t} = v\lambda, \quad (17)$$

$$\frac{\partial B(y, t)}{\partial x} = \lim_{\Delta t \rightarrow 0} \frac{(x-y)^2 f(x, t+\Delta t; y, t)}{\Delta t} = 2D\lambda. \quad (18)$$

Now Eq. (10) can be expanded to the following expression with the first derivative

$$\begin{aligned} & \frac{\partial f(x, t|y, s)}{\partial t} \\ &= -\frac{\partial A(y, t)}{\partial x} f(x, t|y, s) - \frac{\partial f(x, t|y, s)}{\partial x} A(y, t) \\ &+ \frac{1}{2} \frac{\partial}{\partial x} \left[\frac{\partial B(y, t)}{\partial x} f(x, t|y, s) \right. \\ &\left. + \frac{\partial f(x, t|y, s)}{\partial x} B(y, t) \right]. \end{aligned} \quad (19)$$

Substituting Eqs. (12), (15), (17) and (18) into Eq. (19), we have

$$\begin{aligned} & \frac{\partial f(x, t|y, s)}{\partial t} = -v\lambda \cdot f(x, t|y, s) - v \cdot \frac{\partial f(x, t|y, s)}{\partial x} \\ &+ \frac{1}{2} \frac{\partial}{\partial x} \left[D\lambda \cdot f(x, t|y, s) + D \frac{\partial f(x, t|y, s)}{\partial x} \right]. \end{aligned} \quad (20)$$

Because of the constant values of λ and D , Eq. (20) can be expanded further as

$$\begin{aligned} & \frac{\partial f(x, t|y, t)}{\partial t} = -v\lambda \cdot f(x, t|y, s) - v \cdot \frac{\partial f(x, t|y, s)}{\partial x} \\ &+ \frac{1}{2} D\lambda \frac{\partial f(x, t|y, s)}{\partial x} + \frac{1}{2} D \cdot \frac{\partial^2 f(x, t|y, s)}{\partial x^2}. \end{aligned} \quad (21)$$

Substituting Eqs. (12), (15), (17) and (18) into Eq. (21), we have

$$\begin{aligned} & \frac{\partial f(x, t|y, s)}{\partial t} = -v\lambda \cdot f(x, t|y, s) - v \cdot \frac{\partial f(x, t|y, s)}{\partial x} \\ &+ D\lambda \frac{\partial f(x, t|y, s)}{\partial x} + D \cdot \frac{\partial^2 f(x, t|y, s)}{\partial x^2}. \end{aligned} \quad (22)$$

Define

$$C(x, t) = \int_0^t f(x, t; 0, s) ds, \quad (23)$$

which means that the solute concentration at point x by time t is the accumulation of the probability density of particles that move to the point x from the inlet at every time within the interval of $[0, t]$. Then Eq. (22) transforms to a partial differential equation that the solute concentration should meet, i.e.

$$\begin{aligned} & \frac{\partial C(x, t)}{\partial t} = -v\lambda \cdot C(x, t) - v \cdot \frac{\partial C(x, t)}{\partial x} \\ &+ D\lambda \frac{\partial C(x, t)}{\partial x} + D \cdot \frac{\partial^2 C(x, t)}{\partial x^2}. \end{aligned} \quad (24)$$

The physical meaning of the left term in Eq. (24) is the concentration change of solute particles versus time in a porous unit. On the right side of the above equation, the second and last terms denote the contribution of convective and dispersive fluxes to the transportation of solute particles forward, respectively; while the first and third terms indicate the contribution of solute particles in the convective and dispersive fluxes to the total particles captured in a porous unit, respectively.

To solve this equation conveniently, here some dimensionless variables are introduced to make the physical parameters,

$$\begin{aligned} X &= \frac{x}{L}, \quad T = \frac{vt}{L}, \quad \varepsilon_D = \frac{D}{vL}, \quad C = C(X, T), \\ \Lambda &= \lambda L, \quad T \geq 0, \quad 0 < X < 1, \end{aligned}$$

then the equation is converted to

$$\frac{\partial C}{\partial T} = -\Lambda C + (\Lambda \varepsilon_D - 1) \frac{\partial C}{\partial X} + \varepsilon_D \frac{\partial^2 C}{\partial X^2}. \quad (25)$$

Equation (25) is in the same form as the convective dispersion model with adsorption built on the combined bases of both the mass balance equation and the particle capture kinetics equation.^[10]

In summary, the differential form of the Chapman–Kolmogoroff equation can be converted to the Fokker–Planck equation if there is no jump for the particles described. These particles in the process have continuous sample routes. The Fokker–Planck equation describes a process with a continuous sample route. The probability variables that describe the random movement of solute particles have a definite physical significance associated with parameters in the convective dispersion equation. Considering the physical meanings of spatial derivatives of the drift vector and the diffusion matrix, with the constant particle capture probability, the derived convective dispersion equation with adsorption is in the same form as the one deduced by Altoé on the combined bases of both the mass balance equation and the particle capture kinetics. Thus the Markov properties of the convective dispersion of solute particles are confirmed in the derivative process.

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