Research Report

Non-Local, Memory-Dependent Fractional Diffusion in Nano-Porous Reservoirs

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Problem Statement

Problems in Flow Modeling and a Solution

From a fundamental perspective, a major cause of the modeling and characterization problems in nano-porous formations is the inadequacy of the traditional perceptions to describe the movement of fluid molecules in

- extremely small confinement
- spatially disordered media and
- the fractal geometry of the cascade and the scales of natural fractures

Recently, anomalous diffusion has received attention in the context of stochastic physics to describe many physical scenarios similar to those in unconventional reservoirs

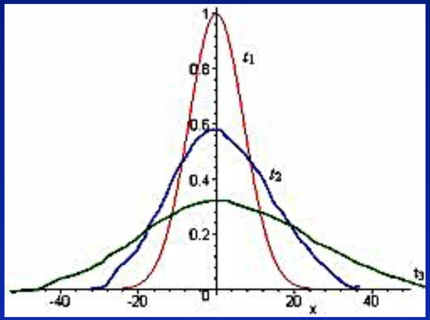
Diffusion

Diffusion is the result of the random Brownian motion of individual particles.

The mean square displacement of a particle is a linear function of time

$$\sigma_r^2 \sim Dt$$

For the Brownian motion, the probability density function in space, evolving in time, is of the Gaussian type



This is a presumption of the use of Laplacian operator

Anomalous Diffusion

However, a convincing number of works have indicated anomalous diffusion in which the mean square variance grows faster (superdiffusion) or slower (subdiffusion) than that in a Gaussian diffusion process.

Thus, a general relationship between the mean square variance and time is given by

$$\sigma_r^2 \sim Dt^{\alpha}$$

$\alpha = 1$ Normal Diffusion
$\alpha \neq 1$ Anomalous Diffusion:
$\alpha > 1$ Superdiffusion
$\alpha < 1$ Subdiffusion.

Physical & Mathematical Basis

Modeling Diffusion

Fick's first law (diffusive flux) for one dimensional diffusion

$$J_C = -D\frac{\partial C}{\partial x}$$

Fick's second law (continuity equation):

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}\left(J_C\right) = \frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x}\right)$$

Defining scaled variables

$$x_D = x/x_0 \qquad t_D = t/t_0 \qquad C_D = C/C_0$$

where x_0, t_0, and C_0 are the characteristics scales, we have

$$\left(\frac{x_0^2}{t_0}\right)\frac{\partial C_D}{\partial t_D} = \frac{\partial}{\partial x_D}\left(D\frac{\partial C_D}{\partial x_D}\right)$$

Modeling Diffusion

Dimensional

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D \frac{\partial C}{\partial x} \right)$$

Dimensionless

$$\left(\frac{x_0^2}{t_0} \right) \frac{\partial C_D}{\partial t_D} = \frac{\partial}{\partial x_D}\left(D \frac{\partial C_D}{\partial x_D} \right)$$

Dimensionless and dimensional diffusion equations are the form if the spatial and temporal scales are related by

$x_0^2 = t_0$ Typical for normal (Fickian) diffusion

For fractal objects, the mean-square displacement of a random walker depends on time as follows:

$$\left\langle x^2 \right\rangle \sim t^{2/(2+\theta)}$$

θ : index of anomalous diffusion ($\theta = 0$ normal diffusion)

Anomalous Diffusion

For normal diffusion $\left\langle x^2 \right\rangle \sim t$ and

Continuity Equation: $$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}\left(J_C\right)$$

Flux Equation: $$J_C = -D\frac{\partial C}{\partial x}$$

For anomalous diffusion (the generalized case), the continuity equation, flux equation, or both should be modified to satisfy

$$\left\langle x^2 \right\rangle \sim t^{2/(2+\theta)} \quad \text{and} \quad \theta = 0 \;\Rightarrow\; \text{normal diffusion}$$

Modeling Anomalous Diffusion

Option 1:

Define $D(x) = D_{f\theta} x^{-\theta}$ $\boldsymbol{D_{f\theta}}$: effective coefficient of diffusion (constant)

Substitution into continuity equation yields

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}\left(J_C\right) = \frac{\partial}{\partial x}\left(D_{f\theta} x^{-\theta} \frac{\partial C}{\partial x}\right)$$

In dimensionless form

$$\frac{x_0^2}{t_0^{2/(2+\theta)}} \frac{\partial C_D}{\partial t_D} = \frac{\partial}{\partial x_D}\left(D_{f\theta} x_D^{-\theta} \frac{\partial C_D}{\partial x_D}\right)$$

which satisfies the scale relation $\left\langle x^2 \right\rangle \sim t^{2/(2+\theta)}$

Modeling Approaches

Option 1:

$$D(x) = D_{f\theta} x^{-\theta} \qquad \frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D_{f\theta} x^{-\theta} \frac{\partial C}{\partial x} \right)$$

The index of anomalous diffusion, *θ*, is determined by the fractal dimension of the medium, d_f.

Example: For the Koch curve (d_f = ln4 / ln3), triple increase in spatial scale creates 16-fold increase in temporal scale:

$$3^{2+\theta} = 16 \Rightarrow 2 + \theta = 2\frac{\ln 4}{\ln 3} = 2d_f \Rightarrow \theta = 2d_f - 2$$

Modeling Approaches

Option 1:

$$D(x) = D_{f\theta} x^{-\theta} \qquad \frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D_{f\theta} x^{-\theta} \frac{\partial C}{\partial x} \right)$$

This approach has been used in petroleum engineering literature to model flow in naturally fractured media; e.g.,

$$\phi(r) \propto r^{d_f - d} \qquad k(r) \propto r^{d_f - d - d_w + 2}$$

Sahimi and Yortsos (1970), Chang and Yortsos (1990), Flamenco-Lopez and Camacho (2003), Camacho et al. (2008), Camacho et al. (2011), etc.

This approach has limitations when we do not have symmetry in the system, etc.

Modeling Approaches

Option 2:

Let β = θ+1 and define a flux proportional to the fractional gradient of concentration of order β

$$J_C = -D_{f\beta} \frac{\partial^\beta C}{\partial x^\beta}$$

Then the dimensional and dimensionless forms of the continuity equation become

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D_{f\beta} \frac{\partial^\beta C}{\partial x^\beta} \right) \qquad \frac{x_0^{1+\beta}}{t_0} \frac{\partial C_D}{\partial t_D} = \frac{\partial}{\partial x_D}\left(D_{f\beta} \frac{\partial^\beta C_D}{\partial x_D^\beta} \right)$$

which satisfy $\left\langle x^2 \right\rangle \sim t^{2/(2+\theta)}$

Modeling Approaches

Option 2:

The new diffusion equation

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D_{f\beta} \frac{\partial^{\beta} C}{\partial x^{\beta}} \right)$$

Note that

$$\frac{\partial}{\partial x}\left(\frac{\partial^{\beta}}{\partial x^{\beta}} \right) = \frac{\partial^{1+\beta}}{\partial x^{1+\beta}} = \frac{\partial^{2+\theta}}{\partial x^{2+\theta}}$$

The order of the spatial derivatives is larger than 2

More than 2 space boundary conditions is required (for θ=0, it does not default to normal diffusion)

Modeling Approaches

Option 2:

To have physically meaningful boundary conditions, the order of the spatial derivative should be 2 or less

This imposes the requirement that $\beta \leq 1$ in

$$J_C = -D_{f\beta} \frac{\partial^\beta C}{\partial x^\beta}$$

$\beta < 1$: non-local spatial gradients (long-range interactions)

To satisfy the scale relation, $\left\langle x^2 \right\rangle \sim t^{2/(2+\theta)}$

the flux relation should also include a fractional temporal derivative (temporal non-locality, memory dependence)

Modeling Approaches

Option 2:

Let us define a new flux relation by

$$J_C = D_{f\gamma\beta}\,\partial_t^{1-\gamma}\left(\frac{\partial^\beta C}{\partial x^\beta}\right), \qquad 0<\gamma, \quad \beta<1$$

where the Caputo definition of the temporal and spatial fractional derivatives are given by

$$\partial_t^\gamma C = \frac{\partial^\gamma C}{\partial t^\gamma} = \frac{1}{\Gamma(1-\gamma)}\int_0^t (t-\xi)^{-\gamma}\frac{\partial C}{\partial \xi}d\xi$$

$$\partial_x^\beta C = \frac{\partial^\beta C}{\partial x^\beta} = \frac{1}{\Gamma(1-\beta)}\int_0^x (x-\xi)^{-\beta}\frac{\partial C}{\partial \xi}d\xi$$

Modeling Approaches

Option 2:

With the new non-local flux, the continuity equation becomes

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left[D_{f\gamma\beta}\, \partial_t^{1-\gamma} \left(\frac{\partial^\beta C}{\partial x^\beta} \right) \right]$$

The scale analysis yields

$$\frac{x_0^{1+\beta}}{t_0^\gamma} \frac{\partial C_D}{\partial t_D} = \frac{\partial}{\partial x_D}\left[D_{f\gamma\beta}\, \partial_{t_D}^{1-\gamma} \left(\frac{\partial^\beta C_D}{\partial x_D^\beta} \right) \right] \rightarrow x_0^2 = t_0^{2\gamma/(1+\beta)}$$

β and *γ* should be such that the the scale relation is satisfied

$$\left\langle x^2 \right\rangle \sim t^{2/(2+\theta)} \rightarrow 2+\theta = (1+\beta)/\gamma$$

Modeling Approaches

Option 2:

Riemann-Liouville fractional integration & derivative of order *α*

$$ {}_aI_t^{\alpha} f(t) = \frac{1}{\Gamma(\alpha)} \int_a^t (t-\tau)^{\alpha-1} f(\tau)\, d\tau $$

$$ {}_a^nD_t^{\alpha} f(t) = \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dt^n} \int_a^t (t-\tau)^{n-\alpha-1} f(\tau)\, d\tau $$

Note that $\partial_t^{\alpha} C = \frac{\partial^{\alpha} C}{\partial t^{\alpha}} = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-\xi)^{-\alpha} \frac{\partial C}{\partial \xi} d\xi = {}_0^1D_t^{\alpha} C$

and the fractional derivative is non-local (it is a convolution; it depends on the values of *C*(*t*) much farther away from *t*)

Modeling Approaches

Option 2:

Applying the Riemann-Liouville fractional integration to both sides of

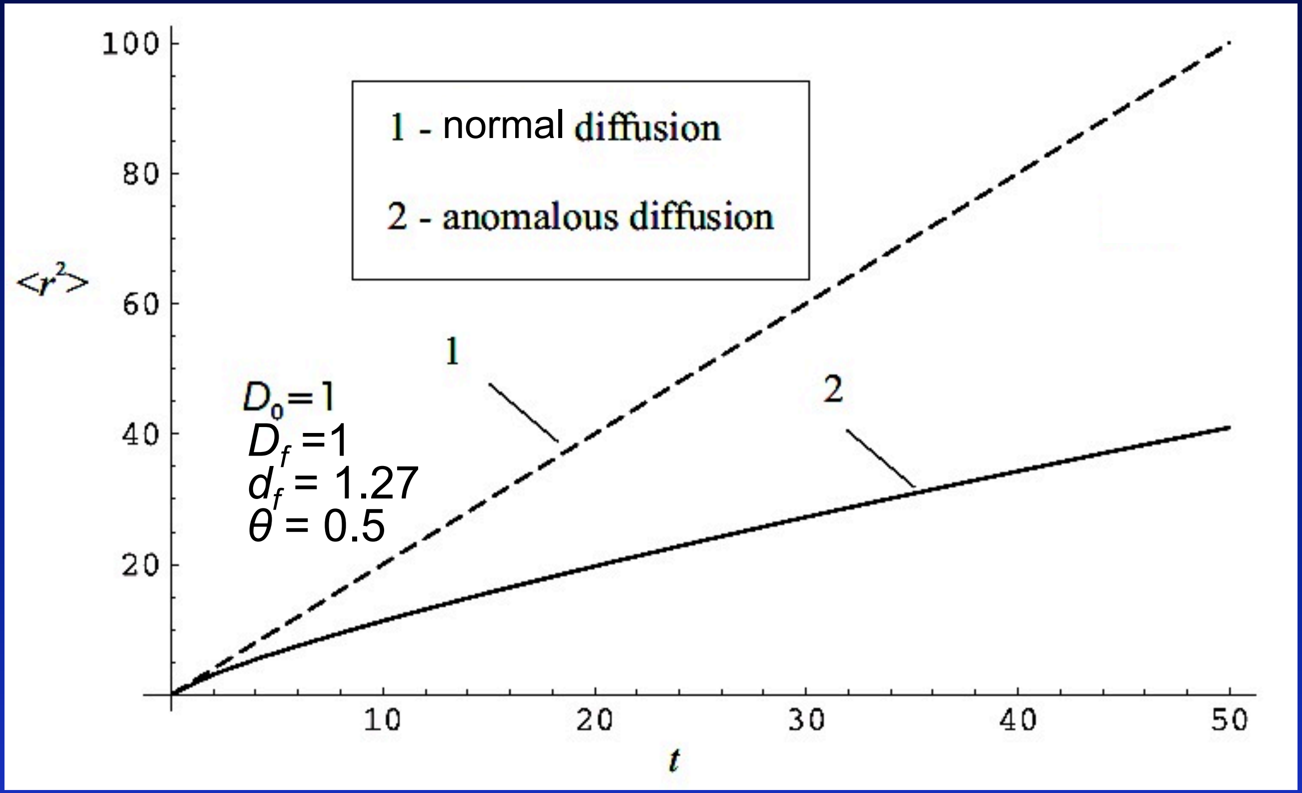
$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left[D_{f\gamma\beta}\, \partial_t^{1-\gamma}\left(\frac{\partial^{\beta} C}{\partial x^{\beta}} \right) \right]$$

we obtain the common form of non-local, time-fractional, anomalous diffusion equation

$$\frac{\partial^{\gamma} C}{\partial t^{\gamma}} = \frac{\partial}{\partial x}\left(D_{f\gamma\beta} \frac{\partial^{\beta} C}{\partial x^{\beta}} \right)$$

Non-Local Anomalous Diffusion

Comparison of mean square displacement vs. time for normal and anomalous diffusion (Fomin et al., 2011)



Non-Local Anomalous Diffusion

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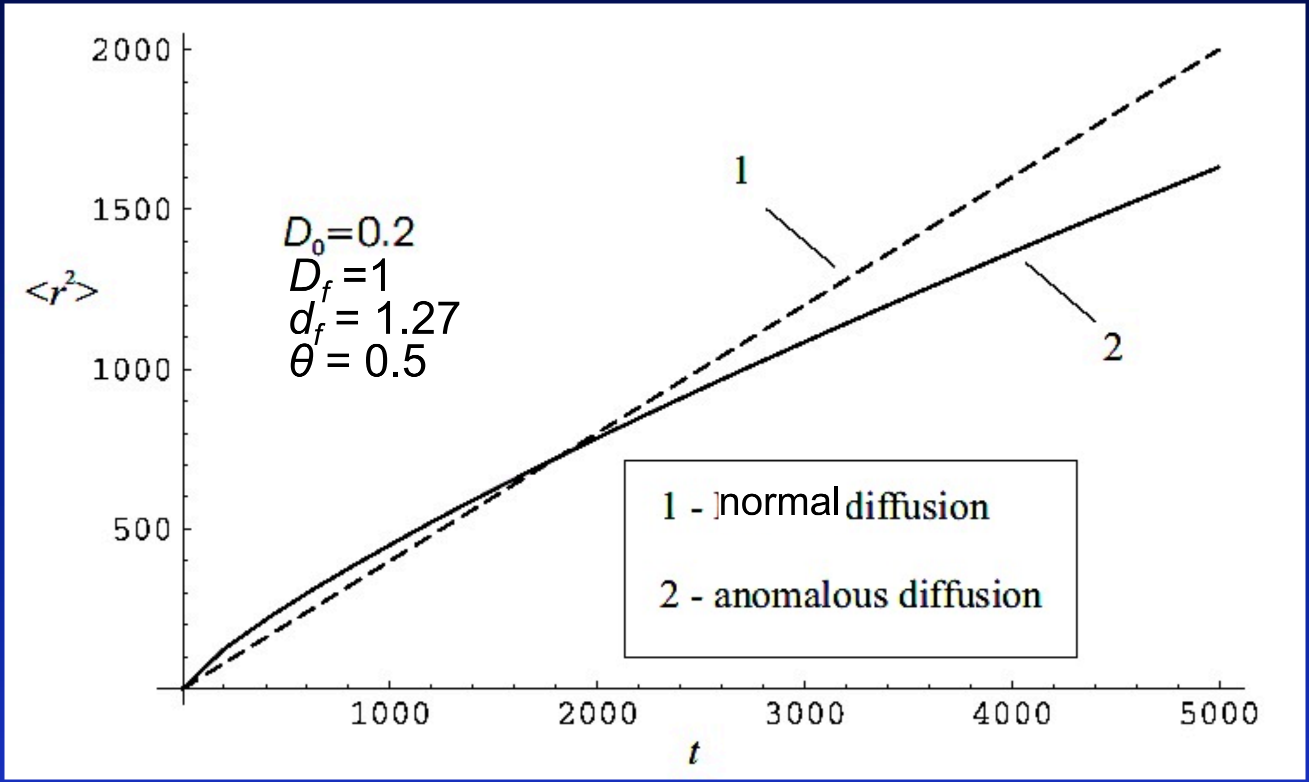

Implications of Anomalous Diffusion

1D Normal Diffusion

Diffusive Flux

$$J_C = -D\frac{\partial C}{\partial x}$$

Continuity Equation):

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x}\right)$$

Integer Derivative

$$\frac{\partial C}{\partial \xi} = \lim_{\Delta\xi \to 0}\frac{C\left(\xi + \Delta\xi\right) - C\left(\xi\right)}{\Delta\xi}$$

Definitions are straightforward

BUT

Characterization is not very successful

Matching the field data is not convincing

1D Non-Local Anomalous Diffusion

Diffusive Flux

$$J_C = D_{f\gamma\beta}\, \partial_t^{1-\gamma}\left(\frac{\partial^\beta C}{\partial x^\beta}\right)$$

Continuity Equation):

$$\frac{\partial^\gamma C}{\partial t^\gamma} = \frac{\partial}{\partial x}\left(D_{f\gamma\beta} \frac{\partial^\beta C}{\partial x^\beta}\right)$$

$$0 < \gamma, \quad \beta < 1$$

Fractional Derivative

$$\partial_\xi^\gamma C = \frac{\partial^\gamma C}{\partial \xi^\gamma} = \frac{1}{\Gamma(1-\gamma)} \int_0^\xi \left(\xi - \xi'\right)^{-\gamma} \frac{\partial C}{\partial \xi'} d\xi'$$

Fractional derivatives are non-local and memory dependent

Implications of Anomalous Diffusion

What is next?

How does this new perception change reservoir characterization and flow modeling?

$$J_C = D_{f\gamma\beta}\, \partial_t^{1-\gamma} \left(\frac{\partial^\beta C}{\partial x^\beta} \right), \quad \frac{\partial^\gamma C}{\partial t^\gamma} = \frac{\partial}{\partial x} \left(D_{f\gamma\beta} \frac{\partial^\beta C}{\partial x^\beta} \right) \qquad 0 < \gamma, \quad \beta < 1$$

How do you estimate a diffusivity coefficient (or permeability) which is defined by a non-local, memory dependent flux law?

How do we use data to determine the fractional powers of the temporal and spatial derivatives?

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