Research Summary

Numerical Modeling of 1D Anomalous Diffusion

Ralf Holy
Colorado School of Mines

Agenda

- Background
- Research Objectives
- Model Updates – Boundary Conditions
- Preliminary Results
- Next Steps

Background

- Classic Diffusion based on Brownian Motion is not adequate to describe fluid flow in ultra tight, highly heterogeneous media due to the presence of:
  - Multi-scale & discontinuous fractures
  - Complex nano-porous matrix

- The use of dual-porosity models requires:
  - Large amounts of measurements at all scales
  - Excessive Discretization of the studied system

Background

- Anomalous Diffusion models via Fractional Calculus can provide an efficient way :
  - To describe multi-scale heterogeneity in complex media (intrinsic property of the fractional derivative)
  - To capture dynamic processes influencing fluid flow on large space & time ranges

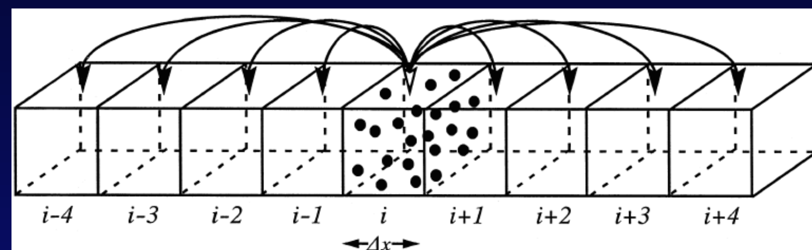
- General 1D Fractional Diffusion Equation in space & time:

$$D_{\alpha,\beta}\frac{\partial^{1+\beta}u(x,t)}{\partial x^{1+\beta}}=\frac{\partial^{\alpha}u(x,t)}{\partial t^{\alpha}} \quad , \ 0<\alpha<1 \ , \ 0<\beta<1$$

$D_{\alpha,\beta}$ ... *anomalous diffusion coefficient*

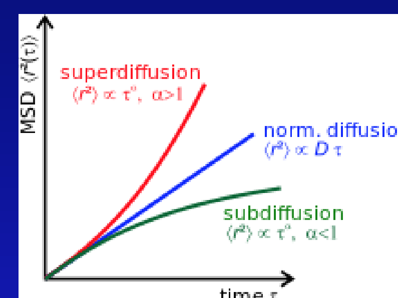
Background

- Influence of space fractional derivative $\frac{\partial^{1+\beta} u(x,t)}{\partial x^{1+\beta}}, \; 0 < \beta < 1$
  - Superdiffusion due to particles ' jumping' to locations further away from current position



Schumer et al. 2001

- Influence of time fractional derivative $\frac{\partial^{\alpha} u(x,t)}{\partial t^{\alpha}}, \; 0 < \alpha < 1$
  - Subdiffusion due to particle being dependent on past time steps (memory effect)
  - Mean square displacement non-linear function of time



Wikipedia

Research Objective

- Derive & implement numerical model incorporating anomalous diffusion in order to better describe & capture the flow of hydrocarbons in ultra tight unconventional media
- Make physical meaning of fractional exponents and anomalous diffusion coefficient
- Examine possibilities to determine the fractional exponents and anomalous diffusion coefficient from experiments

Model – Anomalous Diffusion Equation

Modified Flux Law

$$\vec{u} = -\frac{\bar{\bar{k}}_{\alpha,\beta}}{\mu_o}\frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\nabla^{\beta}P_o \quad , \ 0 < \alpha < 1 \quad , \ 0 < \beta < 1$$

Mass Conservation

$$-\nabla \cdot \left(\frac{\vec{u}}{B_o}\right) = \frac{\phi c_t}{B_o}\frac{\partial P_o}{\partial t}$$

Anomalous Diffusion Equation in Space & Time

$$\nabla \cdot \left(\frac{1}{B_o}\frac{\bar{\bar{k}}_{\alpha,\beta}}{\mu_o}\frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\nabla^{\beta}P_o\right) = \frac{\phi c_t}{B_o}\frac{\partial P_o}{\partial t}$$

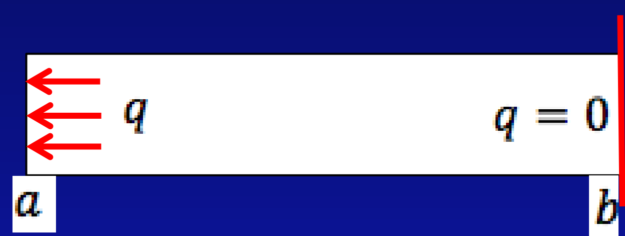
Slightly compressible fluid, constant properties, 1-D

$$\frac{\partial^{1+\beta}P_o}{\partial x^{1+\beta}} = \frac{\phi\mu_o c_t}{k_{\alpha,\beta}}\frac{\partial^{\alpha}P_o}{\partial t^{\alpha}}$$

Model – Anomalous Diffusion Equation

Initial Boundary Value Problem

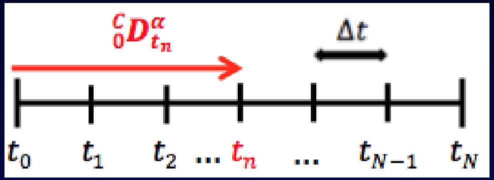
$$
\begin{cases}
\dfrac{\partial^{1+\beta} P_o}{\partial x^{1+\beta}} = \dfrac{\phi \mu_o c_t}{k_{\alpha,\beta}} \dfrac{\partial^{\alpha} P_o}{\partial t^{\alpha}} & for\ a < x < b,\ \ t > 0 \\
P_o(x,0) = P_{o,initial} & for\ a \le x \le b \\
q = -\dfrac{k_{\alpha,\beta} A}{\mu_o} \dfrac{\partial^{1-\alpha}}{\partial t^{1-\alpha}} \left(\dfrac{\partial^{\beta} P_o(a,t)}{\partial x^{\beta}} \right) & for\ t \ge 0 \quad (constant\ rate\ boundary) \\
\dfrac{\partial^{1-\alpha}}{\partial t^{1-\alpha}} \left(\dfrac{\partial^{\beta} P_o(b,t)}{\partial x^{\beta}} \right) = 0 & for\ t \ge 0 \quad (no-flux\ boundary)
\end{cases}
$$



Model – Time Fractional Derivative

Using left sided Caputo definition on interval $[0,t_n]$:

$$\frac{\partial^\alpha P_o(x_i,t_n)}{\partial t^\alpha} = {}_0^C D_{t_n}^\alpha P_o(x_i,t_n) = \frac{1}{\Gamma(1-\alpha)} \int_{t_0=0}^{t_n} \frac{\partial P_o(x_i,\tau)}{\partial t} (t_n-\tau)^{-\alpha}\, d\tau$$



Finite Difference Discretization:

$$\frac{\partial^\alpha P_o(x_i,t_n)}{\partial t^\alpha} = \frac{1}{\Gamma(1-\alpha)} \sum_{k=1}^{n} \int_{(k-1)\Delta t}^{k\Delta t} \frac{P_{o\,i}^{\,k} - P_{o\,i}^{\,k-1}}{\Delta t} (t_n-\tau)^{-\alpha}\, d\tau$$

$$= \frac{1}{\Gamma(1-\alpha)} \sum_{k=1}^{n} \frac{P_{o\,i}^{\,k} - P_{o\,i}^{\,k-1}}{\Delta t} \int_{(k-1)\Delta t}^{k\Delta t} (t_n-\tau)^{-\alpha}\, d\tau$$

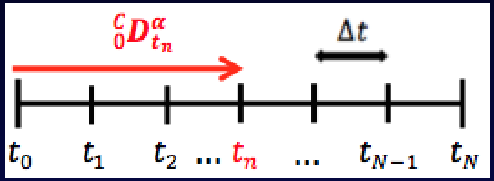
$$= \frac{1}{\Gamma(1-\alpha)} \sum_{k=1}^{n} \frac{P_{o\,i}^{\,k} - P_{o\,i}^{\,k-1}}{\Delta t} \left[-\frac{(t_n-\tau)^{1-\alpha}}{1-\alpha} \right]_{(k-1)\Delta t}^{k\Delta t}$$

$$= \frac{1}{\Gamma(2-\alpha)} \frac{1}{\Delta t^\alpha} \sum_{k=1}^{n} \left(P_{o\,i}^{\,k} - P_{o\,i}^{\,k-1}\right)\left[(n-k+1)^{1-\alpha} - (n-k)^{1-\alpha}\right]$$

Model – Time Fractional Derivative

Compact form after rearranging:

$$\frac{\partial^\alpha P_o(x_i, t_n)}{\partial t^\alpha} = \sigma_{\alpha,\Delta t} \sum_{k=1}^{n} \omega_k^{(\alpha)} \left({P_o}_i^{n+1-k} - {P_o}_i^{n-k} \right)$$



where:

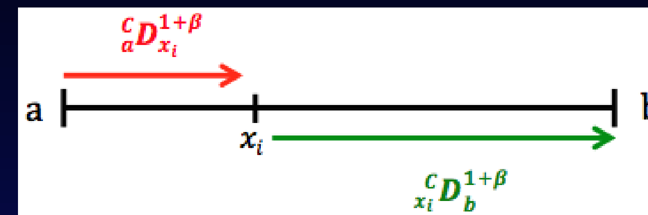
$$\sigma_{\alpha,\Delta t} = \frac{1}{\Gamma(2-\alpha)} \frac{1}{\Delta t^\alpha}$$

$$\omega_k^{(\alpha)} = k^{1-\alpha} - (k-1)^{1-\alpha}$$

Model – Space Fractional Derivative

Using 2-sided Caputo Derivative:

$$\frac{\partial^{1+\beta}}{\partial x^{1+\beta}} P_o(x_i, t_n) = \frac{1}{2}\left({}_a^C D_{x_i}^{1+\beta} + {}_{x_i}^C D_b^{1+\beta} \right), \quad 0 < \beta < 1$$



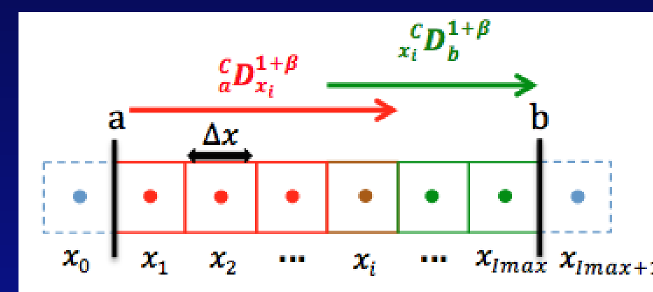
- Left Sided Derivative

$$ {}_a^C D_{x_i}^{1+\beta} = \frac{1}{\Gamma(2-(1+\beta))} \int_a^{x_i} \frac{\partial^2 P_o(\xi, t_n)}{\partial x^2} (x_i - \xi)^{1-(1+\beta)} \, d\xi$$

- Right Sided Derivative

$$ {}_{x_i}^C D_b^{1+\beta} = \frac{(-1)^2}{\Gamma(2-(1+\beta))} \int_{x_i}^{b} \frac{\partial^2 P_o(\xi, t_n)}{\partial x^2} (\xi - x_i)^{1-(1+\beta)} \, d\xi$$

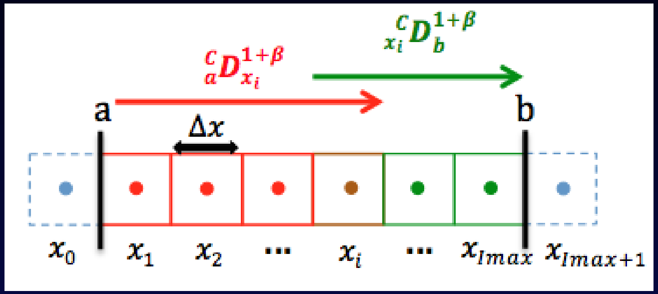
Uniform Grid



Model – Space Fractional Derivative

Finite Difference Discretization:

- Left Sided Derivative



$$ {}_a^C D_{x_i}^{1+\beta} = \frac{1}{\Gamma(2-(1+\beta))}\int_a^{x_i} \frac{\partial^2 P_o(\xi,t_n)}{\partial x^2}(x_i-\xi)^{1-(1+\beta)}\,d\xi $$

$$ = \frac{1}{\Gamma(2-(1+\beta))}\sum_{m=1}^{i}\int_{(m-1)\Delta x}^{m\Delta x}\frac{\left(P_{o\,m+1}^{\;n}-2P_{o\,m}^{\;n}+P_{o\,m-1}^{\;n}\right)}{\Delta x^2}(x_i-\xi)^{1-(1+\beta)}\,d\xi $$

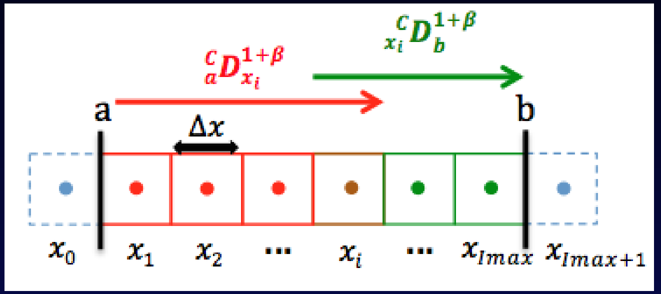
$$ = \frac{1}{\Gamma(2-(1+\beta))}\sum_{m=1}^{i}\frac{\left(P_{o\,m+1}^{\;n}-2P_{o\,m}^{\;n}+P_{o\,m-1}^{\;n}\right)}{\Delta x^2}\left[\frac{-(x_i-\xi)^{2-(1+\beta)}}{2-(1+\beta)}\right]_{(m-1)\Delta x}^{m\Delta x} $$

$$ = \frac{1}{\Gamma(3-(1+\beta))}\frac{1}{\Delta x^{1+\beta}}\sum_{m=1}^{i}\left(P_{o\,m+1}^{\;n}-2P_{o\,m}^{\;n}+P_{o\,m-1}^{\;n}\right)\left[(i-m+1)^{2-(1+\beta)}-(i-m)^{2-(1+\beta)}\right] $$

Model – Space Fractional Derivative

Compact form after rearranging:

$$ {}_{a}^{C}D_{x_i}^{1+\beta} = \sigma_{\beta,\Delta x} \sum_{m=1}^{i} \omega_m^{(\beta)} \left(P_{o\,i+2-m}^{\,n} - 2P_{o\,i+1-m}^{\,n} + P_{o\,i-m}^{\,n} \right) $$



- Right Sided Derivative (Same Approach)

$$ {}_{x_i}^{C}D_b^{1+\beta} = \sigma_{\beta,\Delta x} \sum_{m=1}^{I_{max}-i+1} \omega_m^{(\beta)} \left(P_{o\,i-2+m}^{\,n} - 2P_{o\,i-1+m}^{\,n} + P_{o\,i+m}^{\,n} \right) $$

$$ \sigma_{\beta,\Delta x} = \frac{1}{\Gamma(2-\beta)} \frac{1}{\Delta x^{1+\beta}} $$

$$ \omega_m^{(\beta)} = m^{1-\beta} - (m-1)^{1-\beta} $$

Hence:

$$ \frac{\partial^{1+\beta}}{\partial x^{1+\beta}} P_o(x_i, t_n) = \frac{\sigma_{\beta,\Delta x}}{2} \left\{ \begin{aligned} & \sum_{m=1}^{i} \omega_m^{(\beta)} \left(P_{o\,i+2-m}^{\,n} - 2P_{o\,i+1-m}^{\,n} + P_{o\,i-m}^{\,n} \right) \\ + & \sum_{m=1}^{I_{max}-i+1} \omega_m^{(\beta)} \left(P_{o\,i-2+m}^{\,n} - 2P_{o\,i-1+m}^{\,n} + P_{o\,i+m}^{\,n} \right) \end{aligned} \right\} $$

Model – Constant Rate Boundary

General Formulation:

$$q(a,t_n) = -\frac{k_{\alpha,\beta}A}{\mu_o}\frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\left(\frac{\partial^\beta P_o(a,t_n)}{\partial x^\beta}\right) \Rightarrow \frac{\partial^\beta P_o(a,t_n)}{\partial x^\beta} = -\frac{\mu_o}{k_{\alpha,\beta}A}\frac{\partial^{-(1-\alpha)}}{\partial t^{-(1-\alpha)}}q(a,t_n)$$

Fractional Time Integral for constant rate:

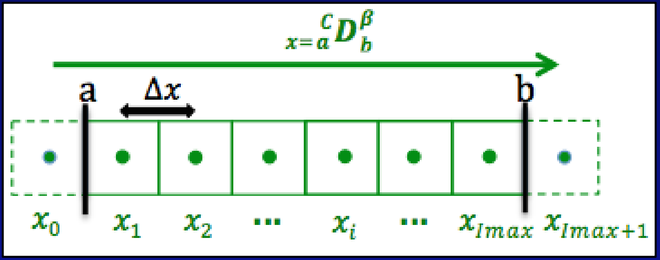
$$\frac{\partial^{-(1-\alpha)}}{\partial t^{-(1-\alpha)}}q = \frac{1}{\Gamma(1-\alpha)}\int_{t_0}^{t_n} q\,(t_n-\tau)^{-\alpha}\,d\tau = \frac{q}{\Gamma(1-\alpha)}\left[\frac{-(t_n-\tau)^{1-\alpha}}{(1-\alpha)}\right]_{t_0}^{t_n} = q\frac{{t_n}^{1-\alpha}}{\Gamma(2-\alpha)} = q\frac{(n\Delta t)^{1-\alpha}}{\Gamma(2-\alpha)}$$

Finite Difference for Right Sided Space Derivative

$$\frac{\partial^\beta P_o(a,t_n)}{\partial x^\beta} = \frac{(-1)^1}{\Gamma(1-\beta)}\int_a^b \frac{\partial P_o(\xi,t_n)}{\partial x}(\xi-a)^{-\beta}\,d\xi$$

$$= \frac{-1}{\Gamma(2-\beta)}\sum_{m=1}^{Imax+1}\frac{{P_o}_m^n - {P_o}_{m-1}^n}{\Delta x}\left[m^{1-\beta}-(m-1)^{1-\beta}\right]\Delta x^{1-\beta}$$

$$= \frac{1}{\Gamma(2-\beta)}\frac{1}{\Delta x^\beta}\sum_{m=1}^{Imax+1}\omega_m^{(\beta)}\left({P_o}_{m-1}^n - {P_o}_m^n\right)$$



$$\omega_m^{(\beta)} = m^{1-\beta} - (m-1)^{1-\beta}$$

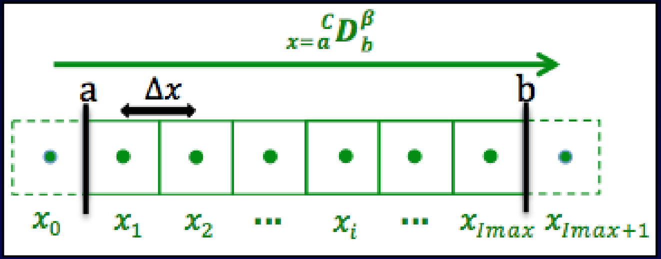
Model – Constant Rate Boundary

Constant Rate Boundary Condition yields:

$$\frac{\partial^\beta P_o(a,t_n)}{\partial x^\beta} = -\frac{\mu_o}{k_{\alpha,\beta}A}\frac{\partial^{-(1-\alpha)}}{\partial t^{-(1-\alpha)}}q(a,t_n)$$

⇩

$$\frac{1}{\Gamma(2-\beta)}\frac{1}{\Delta x^\beta}\sum_{m=1}^{Imax+1}\omega_m^{(\beta)}\left(P_{o\,m-1}^{\,n} - P_{o\,m}^{\,n}\right) = -q\frac{\mu_o}{k_{\alpha,\beta}A}\frac{(n\Delta t)^{1-\alpha}}{\Gamma(2-\alpha)}$$



Hence:

$$\sum_{m=1}^{Imax+1}\omega_m^{(\beta)}\left(P_{o\,m-1}^{\,n} - P_{o\,m}^{\,n}\right) = -q\frac{\mu_o}{k_{\alpha,\beta}A}\frac{(n\Delta t)^{1-\alpha}}{\Gamma(2-\alpha)}\Gamma(2-\beta)\Delta x^\beta$$

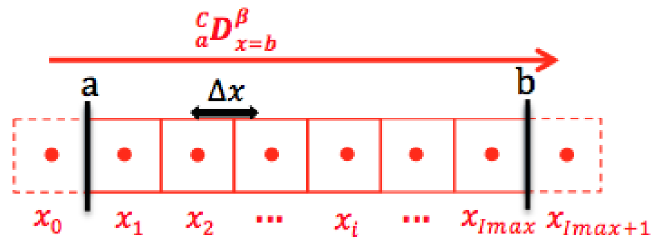
Model – No-Flux Boundary

No-Flux boundary:

$$\frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\left(\frac{\partial^{\beta} P_o(b,t_n)}{\partial x^{\beta}}\right)=0 \;\Rightarrow\; \frac{\partial^{\beta} P_o(b,t_n)}{\partial x^{\beta}}=0$$

Finite Difference for Left Sided Space Derivative

$$\begin{aligned}\frac{\partial^{\beta} P_o(b,t_n)}{\partial x^{\beta}} &= \frac{1}{\Gamma(1-\beta)}\int_a^b \frac{\partial P_o(\xi,t_n)}{\partial x}(b-\xi)^{-\beta}\,d\xi \\ &= \frac{1}{\Gamma(1-\beta)}\sum_{m=1}^{Imax+1}\frac{P_{o\,m}^{\;n}-P_{o\,m-1}^{\;n}}{\Delta x}\left[-\frac{(b-\xi)^{1-\beta}}{1-\beta}\right]_{(m-1)\Delta x}^{m\Delta x} \\ &= \frac{1}{\Gamma(2-\beta)}\frac{1}{\Delta x^{\beta}}\sum_{m=1}^{Imax+1}\omega_m^{(\beta)}\left(P_{o\,Imax+2-m}^{\;n}-P_{o\,Imax+1-m}^{\;n}\right)\end{aligned}$$



Hence:

$$\sum_{m=1}^{Imax+1}\omega_m^{(\beta)}\left(P_{o\,Imax+2-m}^{\;n}-P_{o\,Imax+1-m}^{\;n}\right)=0$$

$$\omega_m^{(\beta)}=m^{1-\beta}-(m-1)^{1-\beta}$$

Model – 1D Implicit Finite Difference Scheme

System of Imax+2 Equations:

- Equation 1:

$$\sum_{m=1}^{Imax+1} \omega_m^{(\beta)} \left(P_{o\,m-1}^{\;n} - P_{o\,m}^{\;n} \right) = -q \frac{\mu_o}{k_{\alpha,\beta} A} \frac{(n\Delta t)^{1-\alpha}}{\Gamma(2-\alpha)} \Gamma(2-\beta) \Delta x^{\beta}$$

- Equation 2 to Imax+1

$$\frac{\sigma_{\beta,\Delta x}}{2} \left\{ \begin{array}{l} \displaystyle\sum_{m=1}^{i} \omega_m^{(\beta)} \left(P_{o\,i+2-m}^{\;n} - 2P_{o\,i+1-m}^{\;n} + P_{o\,i-m}^{\;n} \right) \\ \displaystyle + \sum_{m=1}^{I_{max}-i+1} \omega_m^{(\beta)} \left(P_{o\,i-2+m}^{\;n} - 2P_{o\,i-1+m}^{\;n} + P_{o\,i+m}^{\;n} \right) \end{array} \right\} - \frac{1}{0.006328} \frac{\mu_o \phi c_t}{k_{\alpha,\beta_x}} \sigma_{\alpha,\Delta t} P_{o\,i}^{\;n}$$

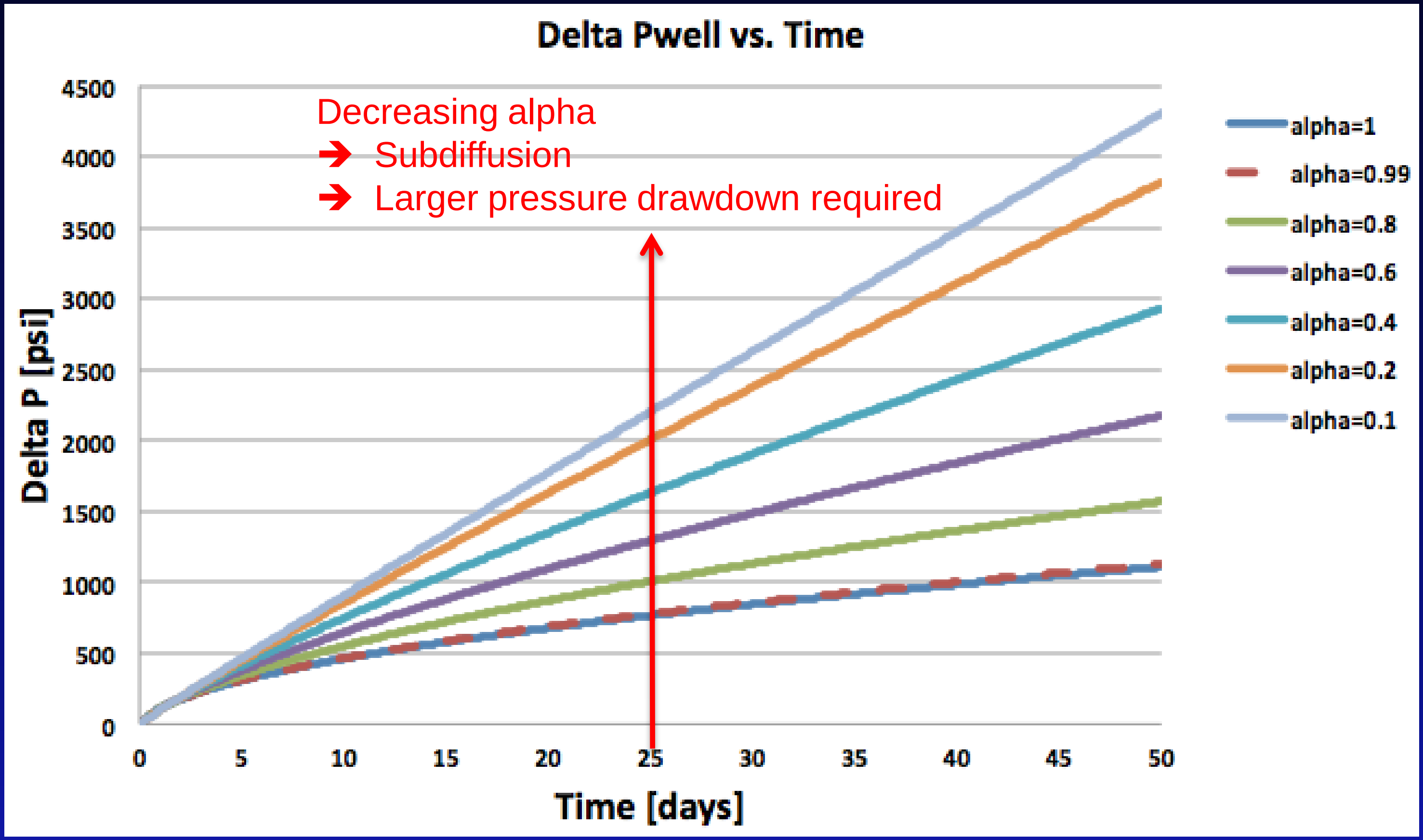
$$= \frac{1}{0.006328} \frac{\mu_o \phi c_t}{k_{\alpha,\beta_x}} \sigma_{\alpha,\Delta t} \left(-P_{o\,i}^{\;n-1} + \sum_{k=2}^{n} \omega_k^{(\alpha)} \left(P_{o\,i}^{\;n+1-k} - P_{o\,i}^{\;n-k} \right) \right)$$

- Equation Imax+2

$$\sum_{m=1}^{Imax+1} \omega_m^{(\beta)} \left(P_{o\,Imax+2-m}^{\;n} - P_{o\,Imax+1-m}^{\;n} \right) = 0$$

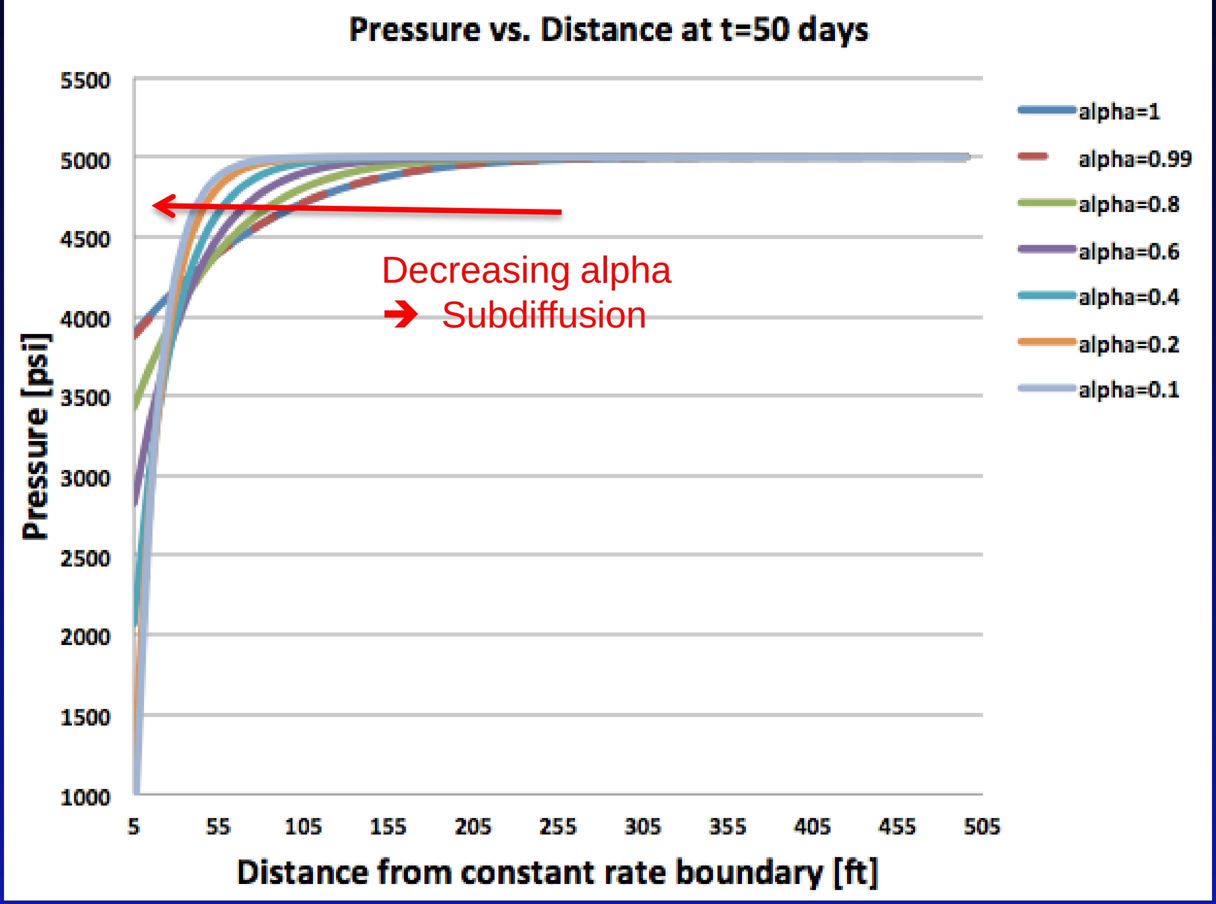
Preliminary Results

Sensitivity Analysis on Time Fractional exponent



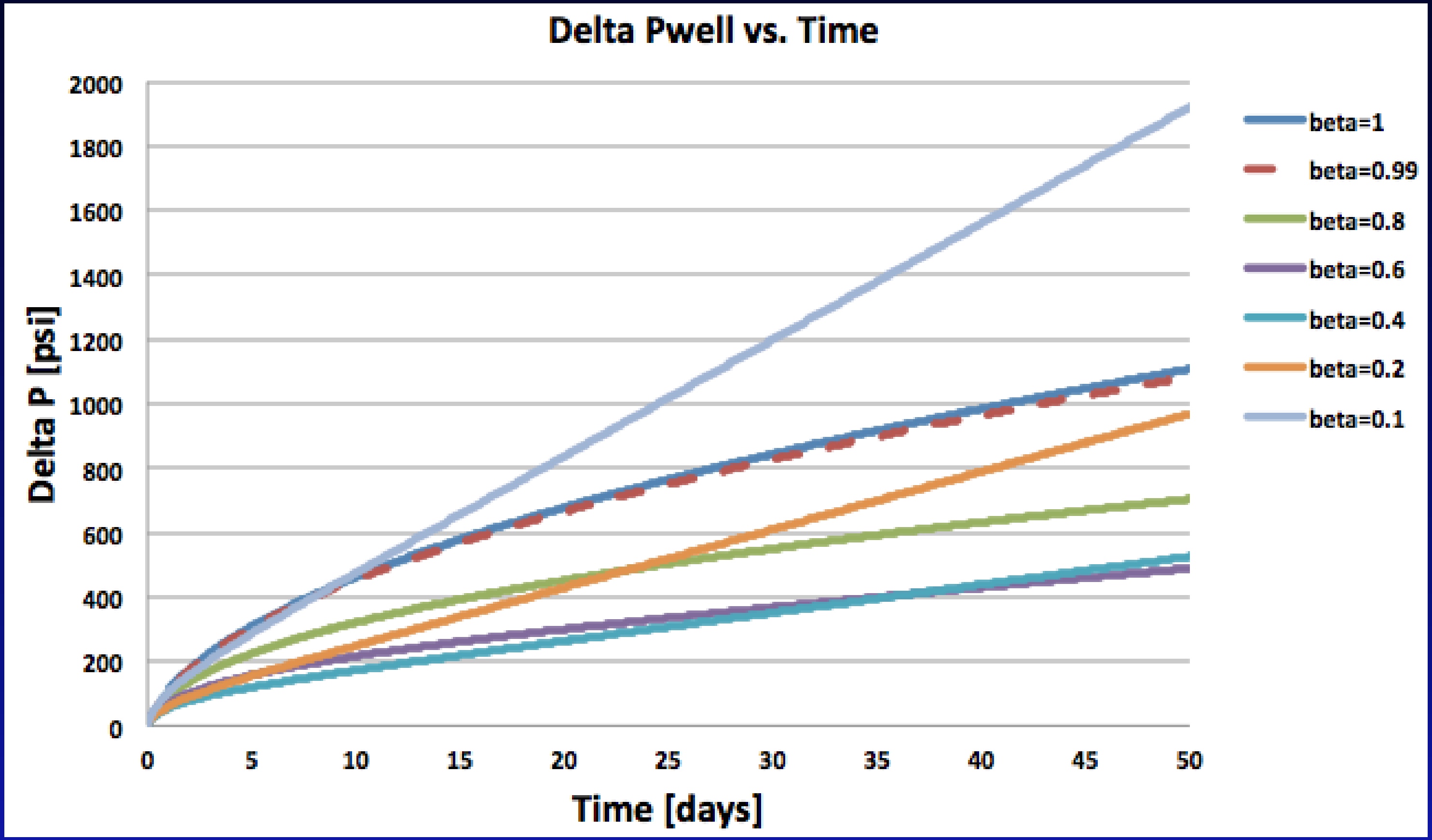
Preliminary Results

Sensitivity Analysis on Time Fractional exponent



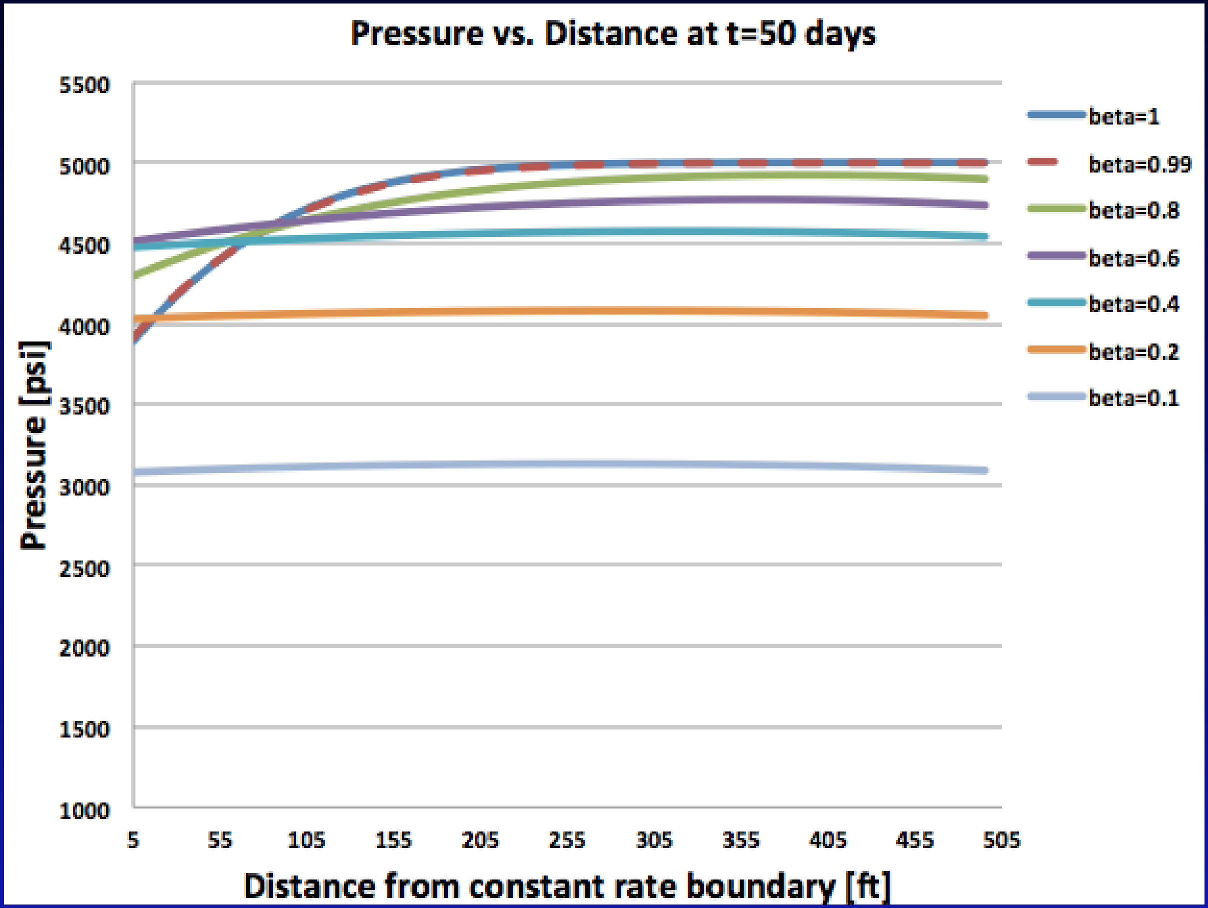
Preliminary Results

Sensitivity Analysis on Space Fractional exponent



Preliminary Results

Sensitivity Analysis on Space Fractional exponent



Next Steps

- Generate dual-porosity model runs for different fracture/matrix property combinations
- Match responses with anomalous diffusion model and assess physical meaning of fractional exponents and ‘anomalous permeability’ coefficient
- Extend model to multiphase
- Explore ways to determine fractional exponents and “anomalous permeability’ through experiments

References

R. Schumer et al., 2000. *Eulerian Derivation of the fractional advection-dispersion equation*. Journal of Contaminant Hydrology 48 (2001) 69-88