Research Summary

Numerical Modeling of Linear Anomalous Diffusion

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Agenda

- Background
- Research Objectives
- Model Derivation
- 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

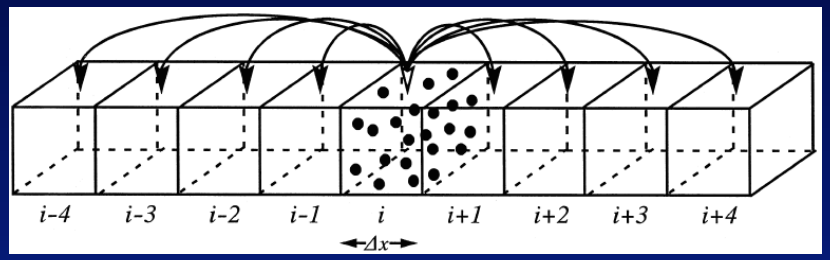
- General 1D Fractional Diffusion Equation in space & time:

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

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

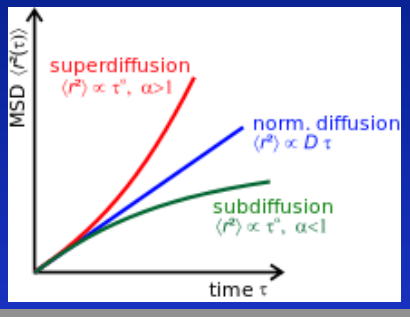
Background

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



Schumer et al. 2001

- Influence of time fractional derivative $\frac{\partial^{\alpha} u(x,t)}{\partial t^{\alpha}}, \quad 0 < \alpha < 1$
  - 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

Single phase, slightly compressible fluid

Modified Flux Law

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

Mass Conservation

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

Anomalous Diffusion Equation in Space & Time

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

Model – Time Fractional Derivative

Finite Difference discretization using left sided implicit Caputo in time:

$$\frac{\partial^\alpha P_o(x,t)}{\partial t^\alpha} = {}^C D^\alpha_{t+}\left(P_o(x,t)\right) = \frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{\frac{\partial P_o(x,\tau)}{\partial t}}{(t-\tau)^\alpha}\,d\tau$$

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

The right hand side of the Anomalous Diff. Eq. becomes:

$$\frac{\emptyset c_t}{B_o}\frac{\partial^\alpha P_o(x,t)}{\partial t^\alpha} = \frac{\emptyset c_t}{B_o}\sigma_{\alpha,\Delta t}\sum_{l=1}^{n}\omega_l^{(\alpha)}\left(P_{o\,i,j}^{\,n+2-l} - P_{o\,i,j}^{\,n+1-l}\right)$$

Where:

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

$$\omega_l^{(\alpha)} = l^{1-\alpha} - (l-1)^{1-\alpha}$$

Model – Time Fractional Integral

Finite Difference discretization using left sided Riemann-Liouville Integral

$$\frac{\partial^{-(1-\alpha)}}{\partial t^{-(1-\alpha)}}\hat{q}_o = I_{t+}^{1-\alpha} = \frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{\hat{q}_o(\tau)}{(t-\tau)^{\alpha}}d\tau = \hat{q}_{o\,i,j}^{\;0}\frac{(n\Delta t)^{1-\alpha}}{\Gamma(2-\alpha)} + \frac{1}{\Gamma(2-\alpha)}\int_0^t \frac{\frac{\partial \hat{q}_o(\tau)}{\partial t}}{(t-\tau)^{\alpha-1}}d\tau$$

$$\cong \hat{q}_{o\,i,j}^{\;0}\frac{(n\Delta t)^{1-\alpha}}{\Gamma(2-\alpha)} + \frac{1}{\Gamma(3-\alpha)}\frac{1}{\Delta t^{\alpha-1}}\sum_{l=1}^{n}\left(\hat{q}_{o\,i,j}^{\;n+2-l} - \hat{q}_{o\,i-l,j}^{\;n+1-l}\right)\left[l^{2-\alpha} - (l-1)^{2-\alpha}\right]$$

For Constant Rate:

$$\frac{\partial^{-(1-\alpha)}}{\partial t^{-(1-\alpha)}}\hat{q}_o = \hat{q}_o\frac{(n\Delta t)^{1-\alpha}}{\Gamma(2-\alpha)}$$

Model – Space Fractional Derivative

1-D Finite Difference discretization using 2-sided Caputo Derivative, assuming uniform grid & constant properties

$$\frac{\partial}{\partial x}\left(\frac{k_{\alpha,\beta_x}}{B_o\mu_o}\frac{\partial^{\beta}P_o}{\partial x^{\beta}}\right)=\frac{k_{\alpha,\beta_x}}{B_o\mu_o}\frac{\partial^{1+\beta}P_o}{\partial x^{1+\beta}}$$

$$\left(\frac{\partial^{1+\beta}P_o}{\partial x^{1+\beta}}\right)_{i,j}^{n+1}=\frac{1}{2}\left({}^{C}D_{x+}^{1+\beta}+{}^{C}D_{x-}^{1+\beta}\right)_{i,j}^{n+1}$$

Left Sided Caputo:

$${}^{C}D_{x+}^{1+\beta}=\frac{1}{\Gamma(2-(1+\beta))}\int_{a}^{x}\frac{\frac{\partial^2 P_o(x,t)}{\partial x^2}}{(x-\xi)^{(1+\beta)-1}}d\xi$$

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

Model – Space Fractional Derivative

Right Sided Caputo:

$$ {}^{C}D_{x+}^{1+\beta} = \frac{1}{\Gamma(2-(1+\beta))}\int_{a}^{x}\frac{\frac{\partial^2 P_o(x,t)}{\partial x^2}}{(x-\xi)^{(1+\beta)-1}}d\xi $$

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

➔ Finite Difference Approximation in space

$$ \left(\frac{\partial^{1+\beta}P_o}{\partial x^{1+\beta}}\right)_{i,j}^{n+1} = \frac{1}{2}\left({}^{C}D_{x+}^{1+\beta}+{}^{C}D_{x-}^{1+\beta}\right)_{i,j}^{n+1} = \frac{1}{2}\left\{\begin{array}{l} \sigma_{\beta,\Delta x}\sum_{l=1}^{i}\omega_l^{(1+\beta)}\left(P_{i+2-l,j}^{n+1}-2P_{i+1-l,j}^{n+1}+P_{i-l,j}^{n+1}\right) \\ +\sigma_{\beta,\Delta x}\sum_{l=1}^{l_{max}-i+1}\omega_l^{(1+\beta)}\left(P_{i-2+l,j}^{n+1}-2P_{i-1+l,j}^{n+1}+P_{i+l,j}^{n+1}\right) \end{array}\right\} $$

where $\sigma_{\beta,\Delta x} = \frac{1}{\Gamma(3-(1+\beta))}\frac{1}{\Delta x^{1+\beta}}$

$$ \omega_l^{(\beta)} = l^{2-(1+\beta)}-(l-1)^{2-(1+\beta)} $$

Model – 1D Implicit Finite Difference Scheme

Multiplying by grid cell volume and rearranging the implicit Finite Difference scheme becomes:

$$T_x \left\{ \begin{array}{l} \displaystyle\sum_{l=1}^{i} \omega_l^{(1+\beta)} \left(P_{i+2-l,j}^{n+1} - 2P_{i+1-l,j}^{n+1} + P_{i-l,j}^{n+1} \right) \\ + \displaystyle\sum_{l=1}^{I_{max}-i+1} \omega_l^{(1+\beta)} \left(P_{i-2+l,j}^{n+1} - 2P_{i-1+l,j}^{n+1} + P_{i+l,j}^{n+1} \right) \end{array} \right\} - VR \frac{\emptyset c_t}{B_o} \sigma_{\alpha,\Delta t} P_{o\,i,j}^{\,n+1}$$

$$= -\frac{Q_o}{B_o} \frac{(n\Delta t)^{1-\alpha}}{\Gamma(2-\alpha)} + VR \frac{\emptyset c_t}{B_o} \sigma_{\alpha,\Delta t} \left\{ -P_{o\,i,j}^{\,n} + \sum_{l=2}^{n} \omega_l^{(\alpha)} \left(P_{o\,i,j}^{\,n+2-l} - P_{o\,i,j}^{\,n+1-l} \right) \right\}$$

Where:

$$T_x = 0.006328 \left(\frac{k_{\alpha,\beta_x}}{B_o \mu_o} \right) VR \frac{\sigma_{\beta,\Delta x}}{2}$$

$$Q_o = \hat{q}_o \Delta x \Delta y \Delta z$$

$$VR = \Delta x \Delta y \Delta z$$

Model – Iteration Matrix

Example:

Iteration Matrix for 1D Problem with 6 grid blocks

$$\begin{bmatrix}
\left(T_x\left(-2\omega_1^{(1+\beta)}+\omega_2^{(1+\beta)}\right)-C\right) & T_x\left(2\omega_1^{(1+\beta)}-2\omega_2^{(1+\beta)}+\omega_3^{(1+\beta)}\right) & T_x\left(\omega_2^{(1+\beta)}-2\omega_3^{(1+\beta)}+\omega_4^{(1+\beta)}\right) & T_x\left(\omega_3^{(1+\beta)}-2\omega_4^{(1+\beta)}+\omega_5^{(1+\beta)}\right) & T_x\left(\omega_4^{(1+\beta)}-2\omega_5^{(1+\beta)}+\omega_6^{(1+\beta)}\right) & T_x\left(\omega_5^{(1+\beta)}-\omega_6^{(1+\beta)}\right) \\
T_x\left(2\omega_1^{(1+\beta)}-\omega_2^{(1+\beta)}\right) & \left(T_x\left(-4\omega_1^{(1+\beta)}+2\omega_2^{(1+\beta)}\right)-C\right) & T_x\left(2\omega_1^{(1+\beta)}-2\omega_2^{(1+\beta)}+\omega_3^{(1+\beta)}\right) & T_x\left(\omega_2^{(1+\beta)}-2\omega_3^{(1+\beta)}+\omega_4^{(1+\beta)}\right) & T_x\left(\omega_3^{(1+\beta)}-2\omega_4^{(1+\beta)}+\omega_5^{(1+\beta)}\right) & T_x\left(\omega_4^{(1+\beta)}-\omega_5^{(1+\beta)}\right) \\
T_x\left(\omega_2^{(1+\beta)}-\omega_3^{(1+\beta)}\right) & T_x\left(2\omega_1^{(1+\beta)}-2\omega_2^{(1+\beta)}+\omega_3^{(1+\beta)}\right) & \left(T_x\left(-4\omega_1^{(1+\beta)}+2\omega_2^{(1+\beta)}\right)-C\right) & T_x\left(2\omega_1^{(1+\beta)}-2\omega_2^{(1+\beta)}+\omega_3^{(1+\beta)}\right) & T_x\left(\omega_2^{(1+\beta)}-2\omega_3^{(1+\beta)}+\omega_4^{(1+\beta)}\right) & T_x\left(\omega_3^{(1+\beta)}-\omega_4^{(1+\beta)}\right) \\
T_x\left(\omega_3^{(1+\beta)}-\omega_4^{(1+\beta)}\right) & T_x\left(\omega_2^{(1+\beta)}-2\omega_3^{(1+\beta)}+\omega_4^{(1+\beta)}\right) & T_x\left(2\omega_1^{(1+\beta)}-2\omega_2^{(1+\beta)}+\omega_3^{(1+\beta)}\right) & \left(T_x\left(-4\omega_1^{(1+\beta)}+2\omega_2^{(1+\beta)}\right)-C\right) & T_x\left(2\omega_1^{(1+\beta)}-2\omega_2^{(1+\beta)}+\omega_3^{(1+\beta)}\right) & T_x\left(\omega_2^{(1+\beta)}-\omega_3^{(1+\beta)}\right) \\
T_x\left(\omega_4^{(1+\beta)}-\omega_5^{(1+\beta)}\right) & T_x\left(\omega_3^{(1+\beta)}-2\omega_4^{(1+\beta)}+\omega_5^{(1+\beta)}\right) & T_x\left(\omega_2^{(1+\beta)}-2\omega_3^{(1+\beta)}+\omega_4^{(1+\beta)}\right) & T_x\left(2\omega_1^{(1+\beta)}-2\omega_2^{(1+\beta)}+\omega_3^{(1+\beta)}\right) & \left(T_x\left(-4\omega_1^{(1+\beta)}+2\omega_2^{(1+\beta)}\right)-C\right) & T_x\left(2\omega_1^{(1+\beta)}-\omega_2^{(1+\beta)}\right) \\
T_x\left(\omega_5^{(1+\beta)}-\omega_6^{(1+\beta)}\right) & T_x\left(\omega_4^{(1+\beta)}-2\omega_5^{(1+\beta)}+\omega_6^{(1+\beta)}\right) & T_x\left(\omega_3^{(1+\beta)}-2\omega_4^{(1+\beta)}+2\omega_5^{(1+\beta)}\right) & T_x\left(\omega_2^{(1+\beta)}-2\omega_3^{(1+\beta)}+\omega_4^{(1+\beta)}\right) & T_x\left(2\omega_1^{(1+\beta)}-2\omega_2^{(1+\beta)}+\omega_3^{(1+\beta)}\right) & \left(T_x\left(-2\omega_1^{(1+\beta)}+\omega_2^{(1+\beta)}\right)-C\right)
\end{bmatrix}_{6\times6}
\begin{bmatrix} P_1 \\ P_2 \\ P_3 \\ P_4 \\ P_5 \\ P_6 \end{bmatrix}^{n+1}$$

Where $C = VR\dfrac{\emptyset c_t}{B_o}\sigma_{\alpha,\Delta t}$

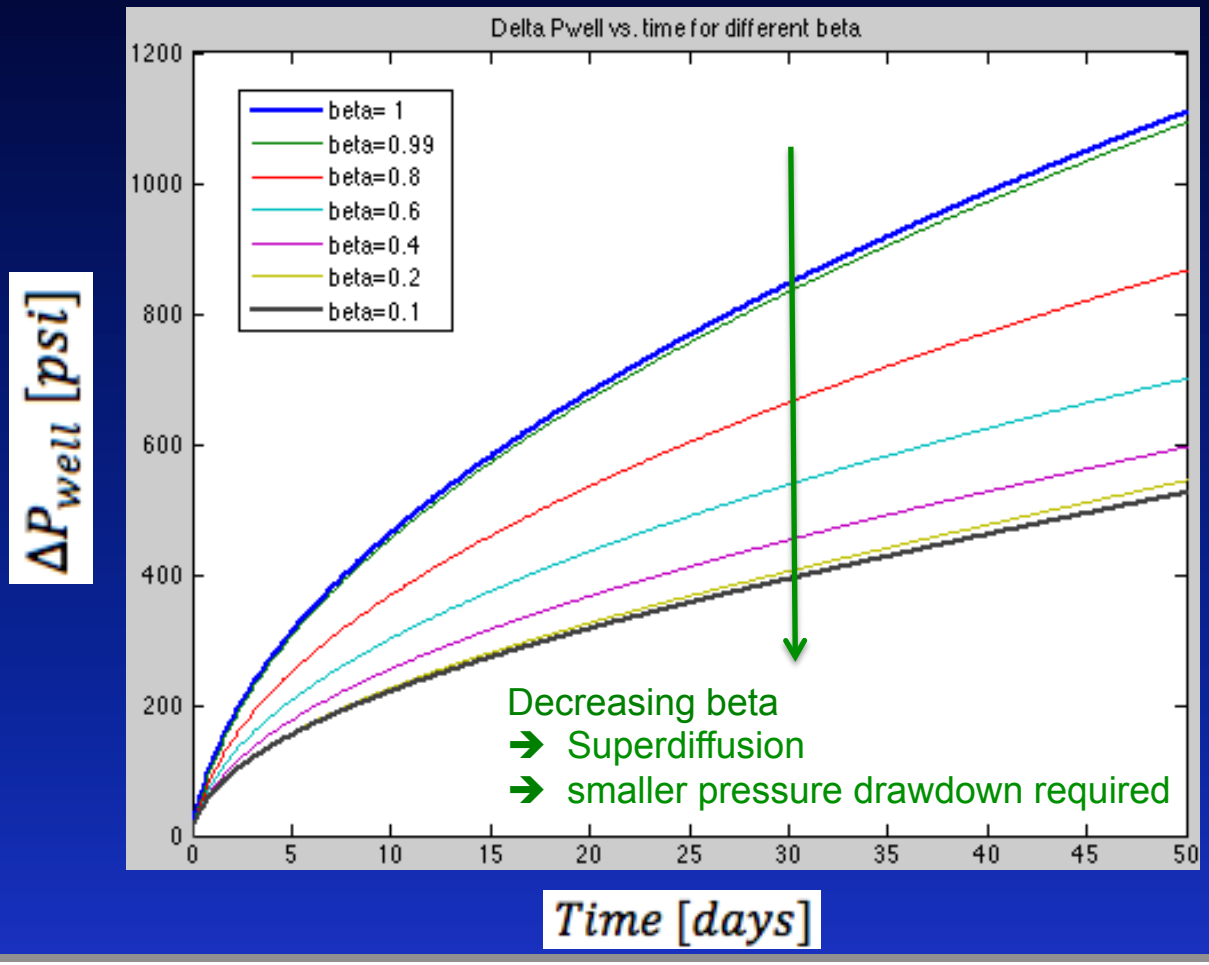
Note:

$$For\ \beta = 1: \quad \omega_1^{(\beta)} = 1\,,\ \ \omega_l^{(\beta)} = 0\ \ for\ l > 1$$

➔ Matrix collapses back to classic tri-diagonal Matrix

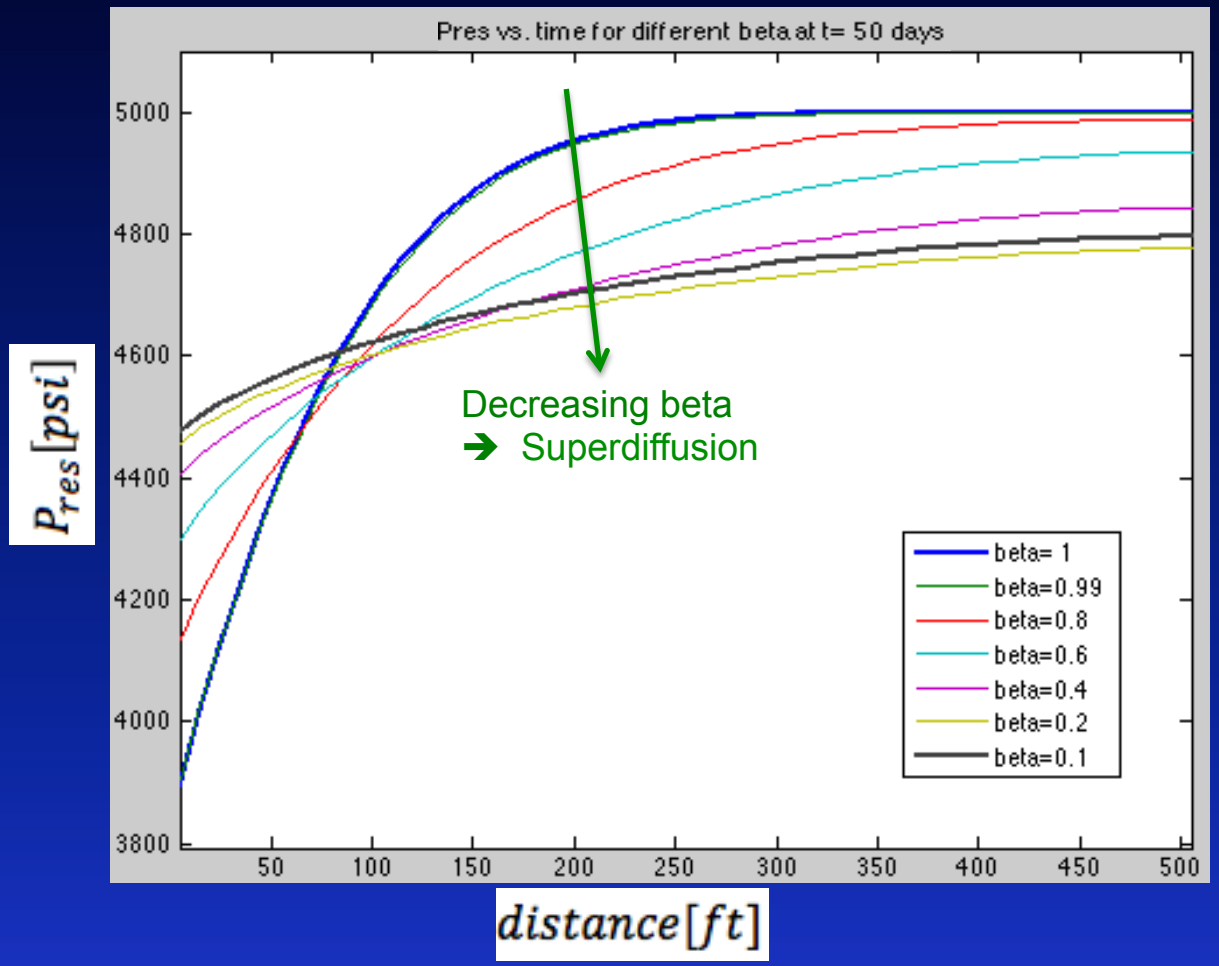
Preliminary Results

Sensitivity Analysis on Space Fractional exponent



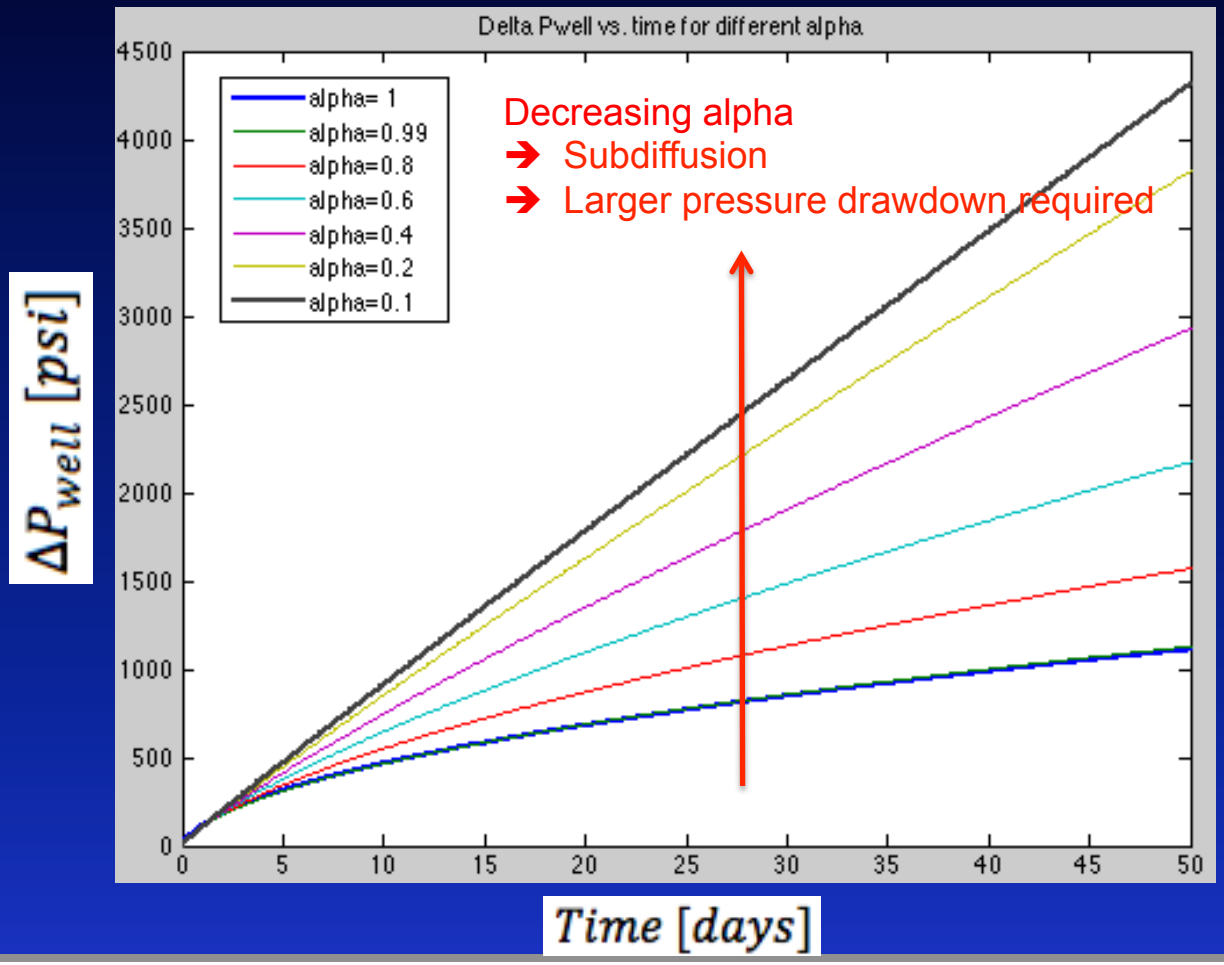
Preliminary Results

Sensitivity Analysis on Space Fractional exponent



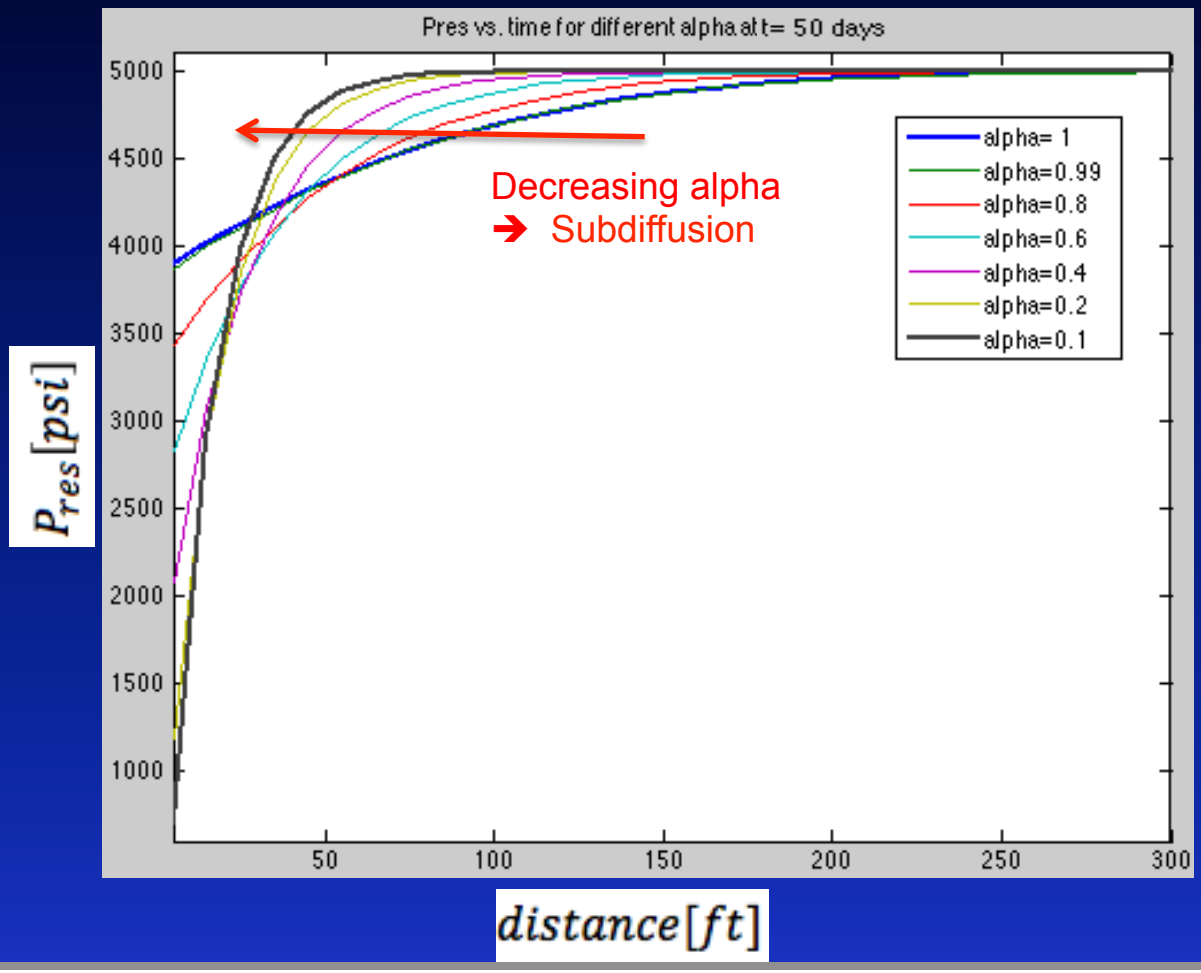
Preliminary Results

Sensitivity Analysis on Time Fractional exponent



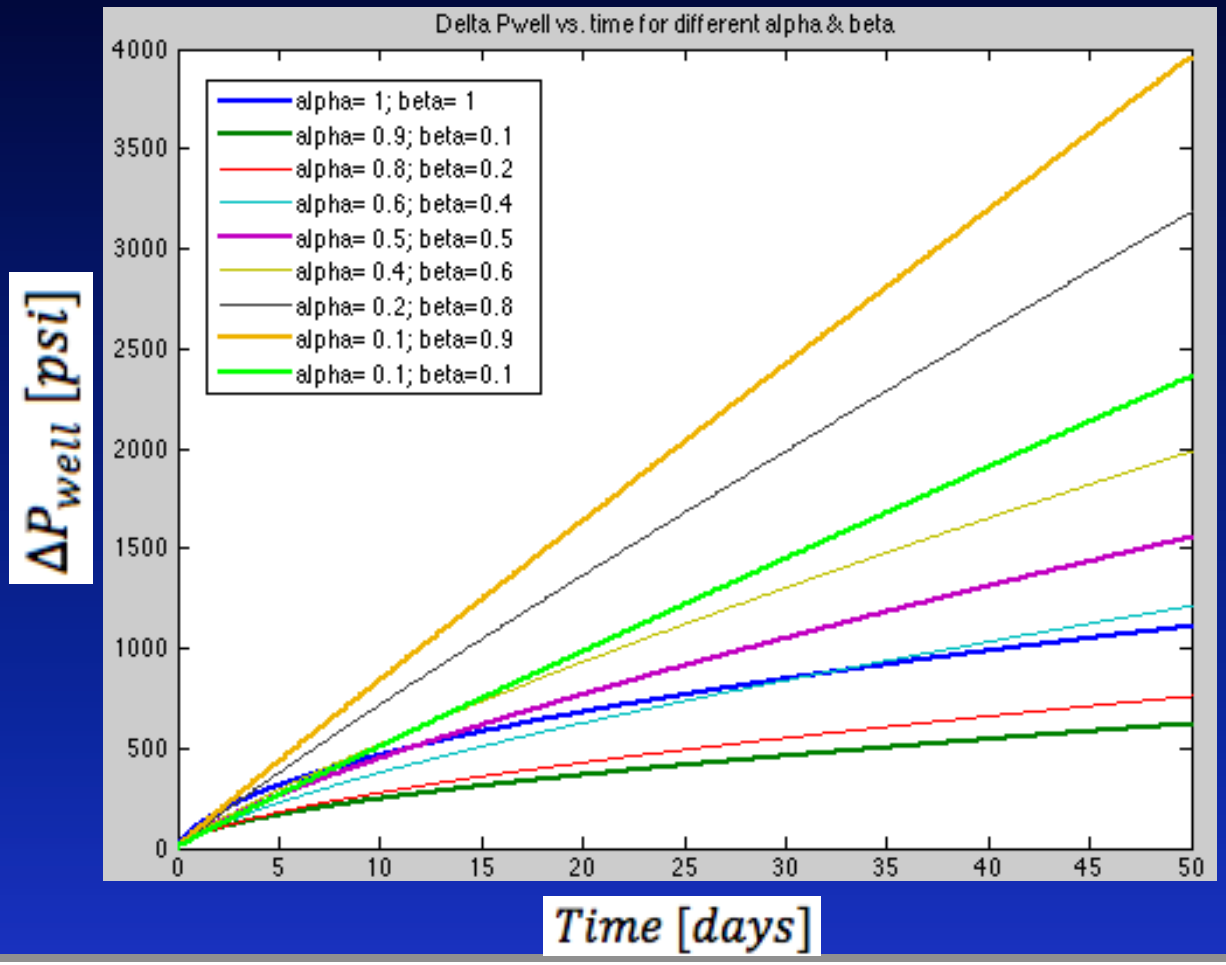
Preliminary Results

Sensitivity Analysis on Time Fractional exponent



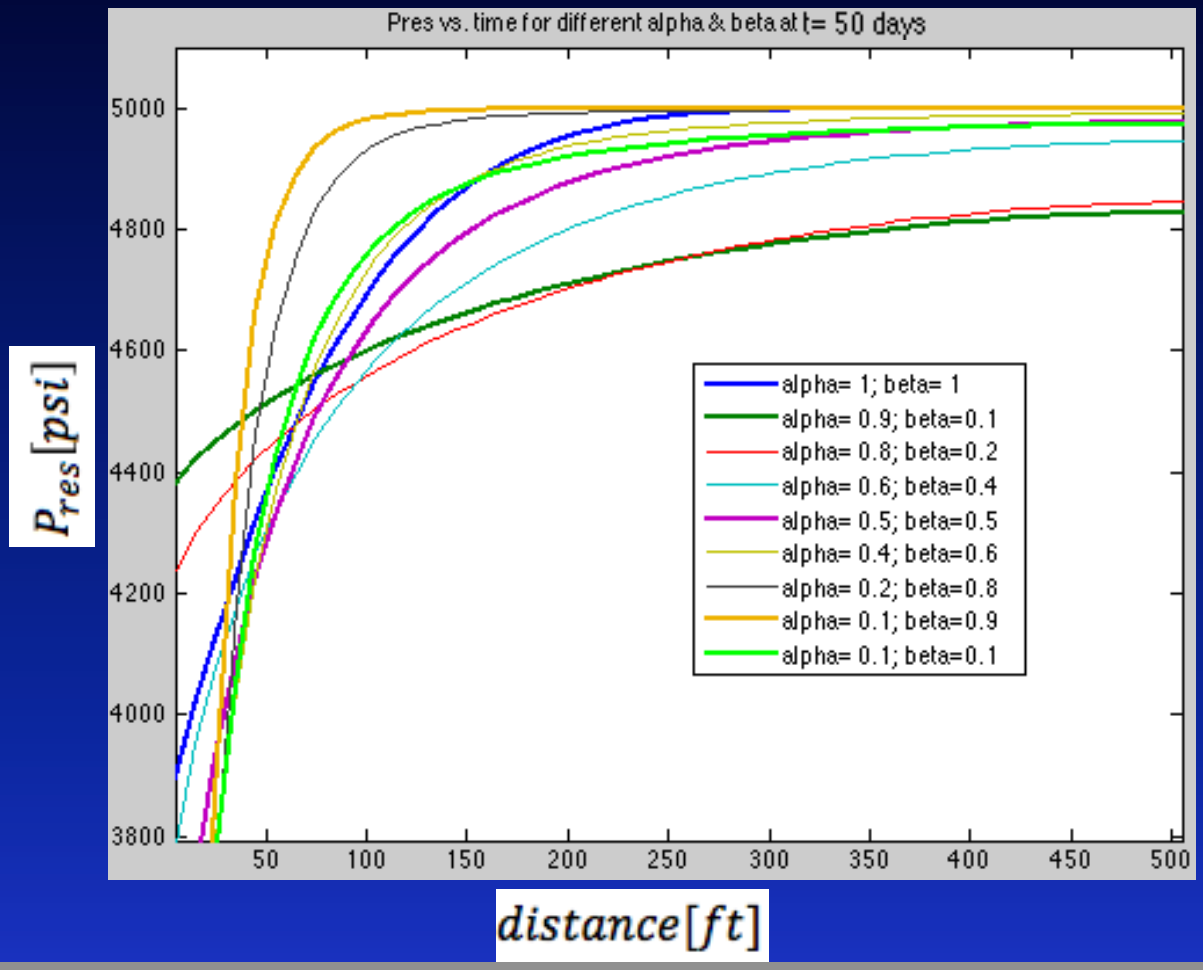
Preliminary Results

Sensitivity Analysis on Space & Time Fractional exponents



Preliminary Results

Sensitivity Analysis on Space & Time Fractional exponents



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 & 2D
- 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