Modeling and Analysis of Transient Well Responses by Anomalous Diffusion

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Agenda

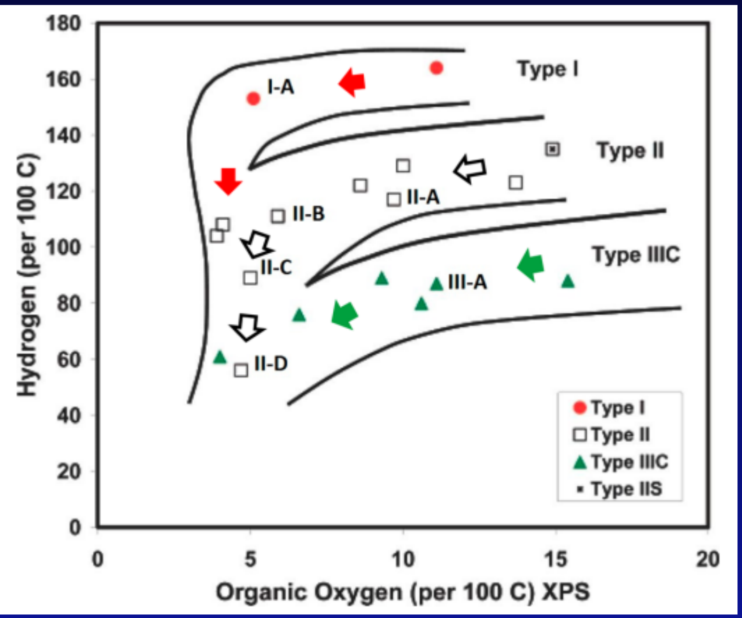
- Motivation & Objective
- Applications of molecular dynamics in oil & gas industry
    - Kerogen maturation
    - Transport diffusivity and adsorption
    - Retrograde condensation
- Anomalous diffusion
    - Brief description
    - Reasons of anomalous diffusion
    - Memory effect
    - Investigating the diffusivity coefficient from molecular dynamics simulations
- Determining diffusion types in an unconventional reservoir using RTA

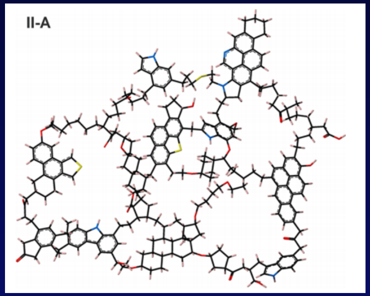
Motivation and Objective

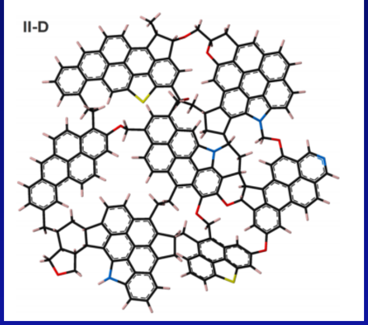
- 1-D Anomalous diffusion numerical model was developed by Ralf Holy (2016)
- Fractional derivatives and flux coefficient include the long-range effects and the memory of the system
    - Robust approaches are needed to determine the anomalous diffusion parameters $\left(\alpha, \beta, k_{\alpha,\beta}\right)$ from field data, cores, simulations, etc.
- In the numerical evaluation of anomalous diffusion, large sums over space and time are required to take into account the long-range and memory effects.
    - Molecular dynamics (MD) simulations may help to determine an optimum distance and time to truncate the series.
- In most applications, $k_{\alpha,\beta}$ is assumed constant
    - We will investigate if the term remains constant
    - If not, how can it be determined?
- There is still need to document the importance of considering anomalous diffusion in unconventional reservoirs

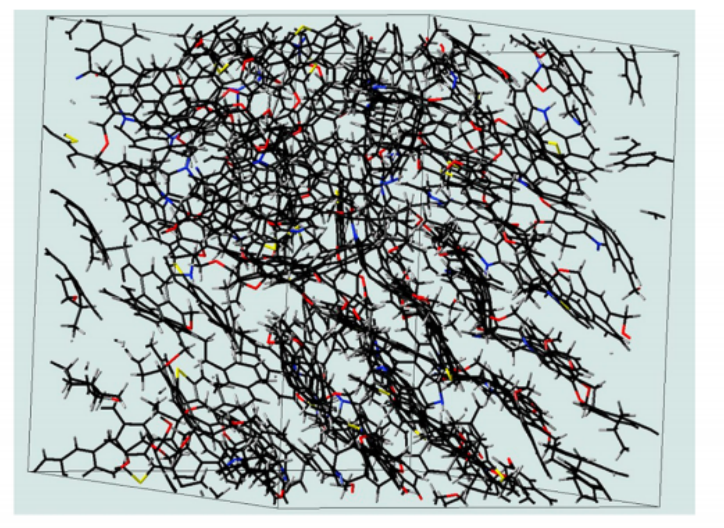
Applications of molecular dynamics

Volumetric and thermodynamic properties of kerogen: influence of organic type and maturity (Ungerer et al. 2014)





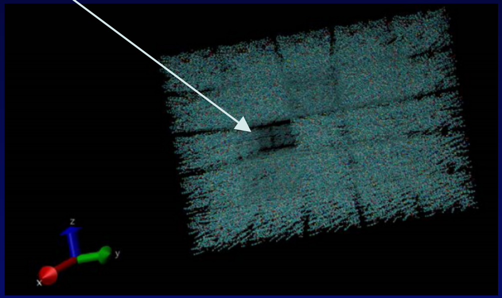




Applications of molecular dynamics

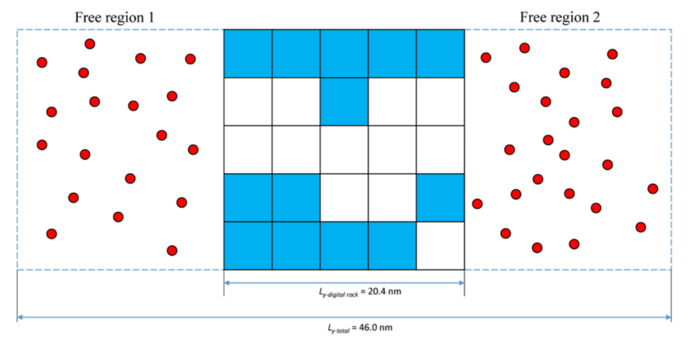
Estimation of transport diffusivity of natural gas in organic matter(He et al. 2016) (SPE 180198)

Pore

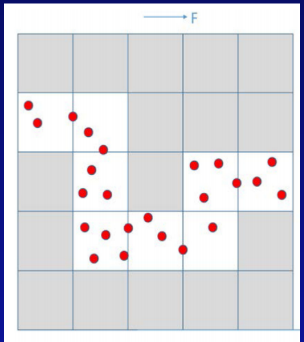


They follow a similar algorithm to Ungerer's work to create a kerogen structure.

In to a digital rock sample containing 5x5x5 voxels, they put the kerogen structure and create a matrix.



Rock Sample 1, before simulation



Rock Sample 2, after simulation

The purpose of the simulations is to measure the amount of CH_4 adsorbed in the porous media as well as the transport diffusivity coefficient.

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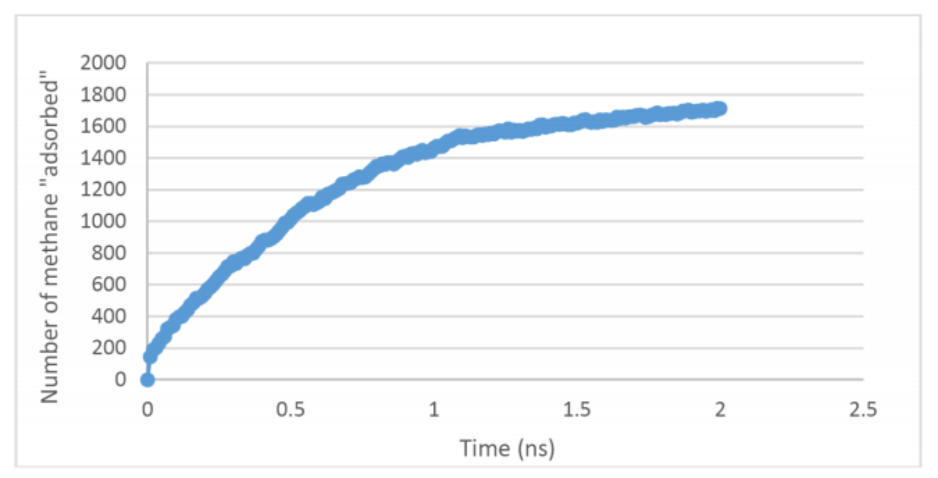
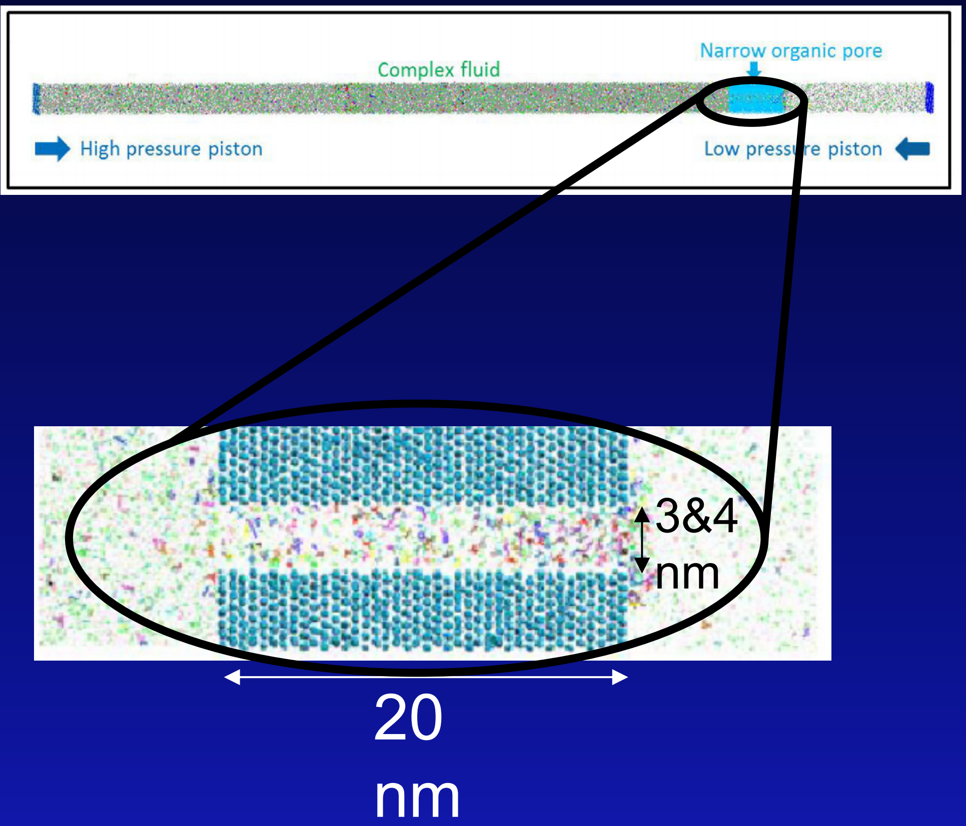


Rock Sample 2					
External Force (Kcal/mol-Å)	**0.3**	**0.5**	**-0.3**	**-0.5**	**average**
Gas Pressure (MPa)	Transprot Diffusivty Coefficient (X 10-8 m2/s)				
7.59	3.87	3.04	4.29	3.61	3.704
13.99	5.75	5.44	6.11	5.75	5.763
24.57	7.70	8.54	8.67	9.34	8.562
28.84	11.92	11.83	11.44	11.98	11.79

Rock Sample 2					
External Force (Kcal/mol-Å)	**0.3**	**0.5**	**-0.3**	**-0.5**	**average**
Gas Pressure (MPa)	Transprot Diffusivty Coefficient (X 10-8 m2/s)				
6.79	4.37	3.49	4.92	4.23	4.253
12.28	6.18	6.02	6.73	6.43	6.339
21.93	8.66	9.53	9.71	10.8	9.675
34.93	13.7	13.9	15.7	18.34	15.43

Applications of molecular dynamics

Retrograde Condensation in Nanoporous Shale (Welch and Piri 2015) (SPE 178682)



A complex fluid is pushed through 3 & 4 nm pore

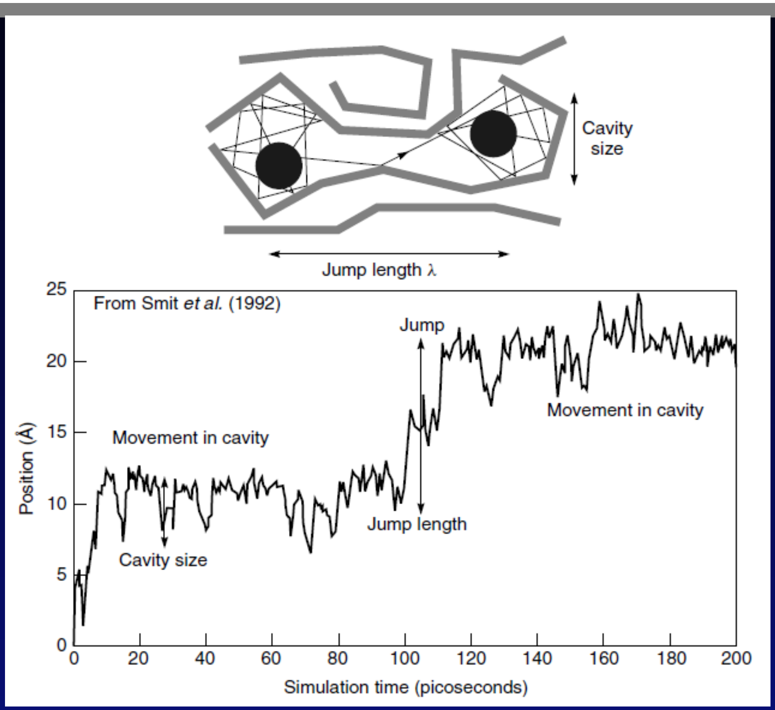
At 3 nm case,

- Capillary condensation seales the pore completely and inhibited flow
- Even high pressure application doesn't open it

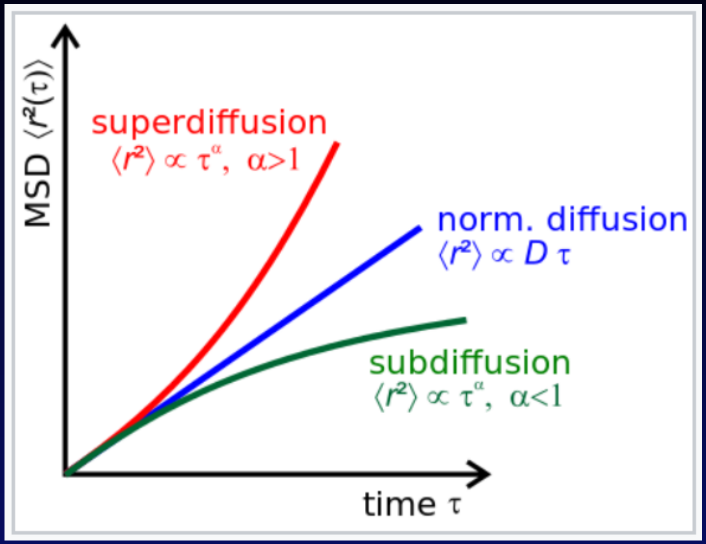
At 4 nm case,

- The pore is not completely sealed and flow is less inhibited
- ❖ Pressure gradient from 400 to 60 bar
- ❖ Accumulation of hydrocarbons occurred in the lower pressure end

Anomalous Diffusion



Baker (2004)



Particle translation from one point to another

α=1 $normal\ diffusion$,
α>1 $super\ diffusion$

Longer particle jump length due to excitations, facilitations
α<1 $subdiffusion$

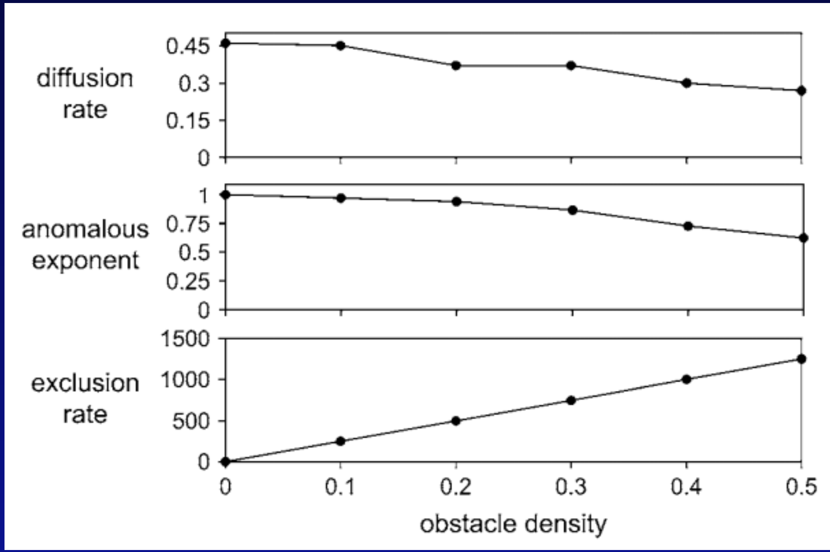
Lower particle jump length due to entrapments, retardations

Sources of Anomalous Diffusion

Nicolau et al. (2007) studied a stochastic random walk model of protein molecule diffusion on a cell membrane to investigate the reasons of anomalous diffusion. They explained the sources as:

- The presence of a significant number of fixed obstacles on the membrane (in their study, the obstacles are immobile proteins, in our study the obstacles are immobile organic matter (kerogen) and minerals)

- The interaction of mobile proteins and lipids with picket posts anchored to membrane skeleton mesh (in our case, the interaction occurs between the mobile hydrocarbon and pore walls containing carbon and minerals



1-D anomalous diffusion

Holy (2018) presented the combination of fractional flux law and mass conservation equation as:

$$\boldsymbol{u}(\boldsymbol{x},\boldsymbol{t}) = -\frac{\boldsymbol{k}_{\boldsymbol{\alpha},\boldsymbol{\beta}}}{\boldsymbol{\mu}}\left(\frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\frac{\partial^{\beta}p(x,t)}{\partial x^{\beta}}\right)$$

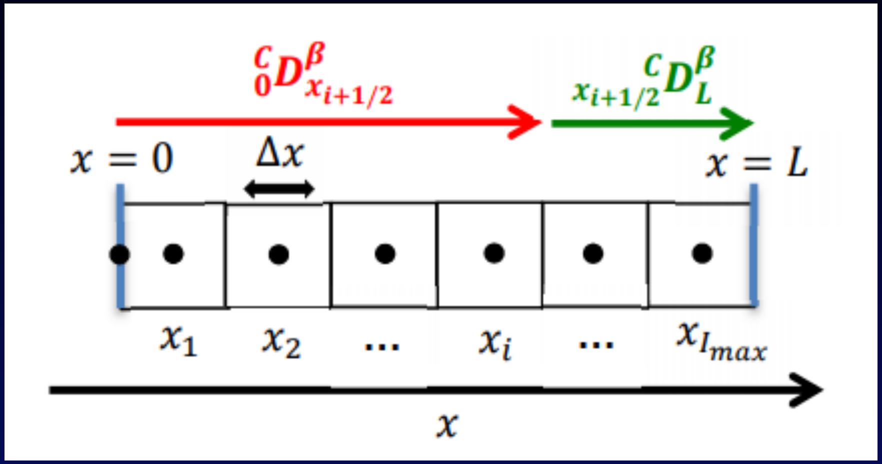
$$\frac{\partial}{\partial x}\frac{\boldsymbol{k}_{\boldsymbol{\alpha\beta}}}{\boldsymbol{\mu}}\left(\frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\frac{\partial^{\beta}p(x,t)}{\partial x^{\beta}}\right) = (\phi c_t)_o\frac{\partial p(x,t)}{\partial t}$$

Having $\alpha = 1$ and $\beta = 1$ we get normal diffusion

$$\frac{\partial}{\partial x}\frac{\boldsymbol{k}}{\boldsymbol{\mu}}\left(\frac{\partial p(x,t)}{\partial x}\right) = (\phi c_t)_o\frac{\partial p(x,t)}{\partial t}$$

α: Time fractional derivative order / sub-diffusion exponent
β: Space fractional derivative order / super diffusion exponent

1-D anomalous diffusion – Memory Effect



From Holy 2017

$$\frac{\partial}{\partial x}(\boldsymbol{u}(\boldsymbol{x},\boldsymbol{t})) = (\phi c_t)_o \frac{\partial p(x,t)}{\partial t}$$

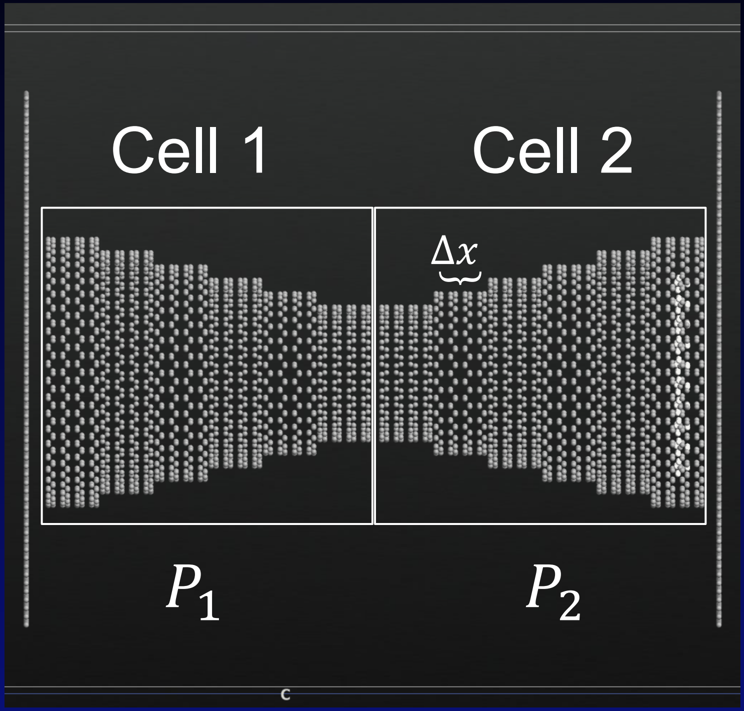
Discretization of above equation gives:

$$\frac{P_i^{n+1} - P_i^n}{\Delta t} \phi_i^n c_t = \frac{1}{\Delta_x}\left([u(x,t)]_{i+\frac{1}{2}}^{n+1} - [u(x,t)]_{i-\frac{1}{2}}^{n+1}\right)$$

$$\left[\frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\left(\frac{\partial^\beta p(x,t)}{\partial x^\beta}\right)\right]_{i\mp 1/2}^{n+1} = \overbrace{\frac{1}{\Gamma(\alpha)}\int_{t_0=0}^{t_{n+1}} \frac{\partial}{\partial \tau}\left(\frac{\partial^\beta p(x_{i\mp 1/2},\tau)}{\partial x^\beta}\right)(t_{n+1}-\tau)^{-(1-\alpha)}d\tau}^{Time\ fractional\ derivative}$$

$$\frac{\partial^\beta p(x_{i\mp 1/2},\tau)}{\partial x^\beta} = \overbrace{\left({}^{C}_{0}D^{\beta}_{x_{i\mp\frac{1}{2}}}\right) * m - \left({}_{x_{i\mp\frac{1}{2}}}{}^{C}D^{\beta}_{L}\right)(1-m)_{x_{i\mp 1/2}}}^{Space\ fractional\ derivative}$$

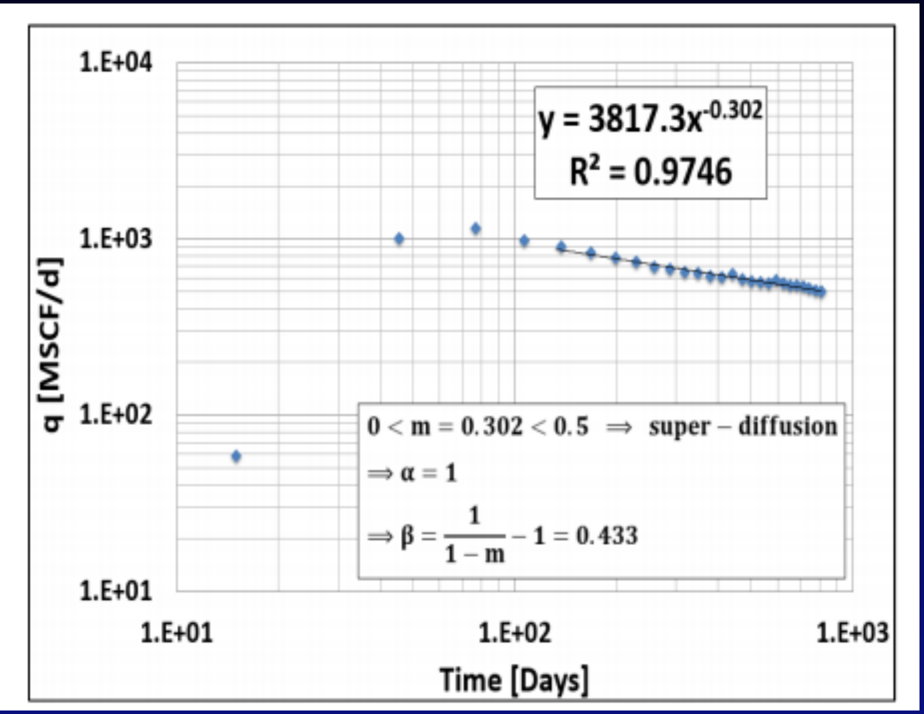
1-D anomalous diffusion – Memory Effect



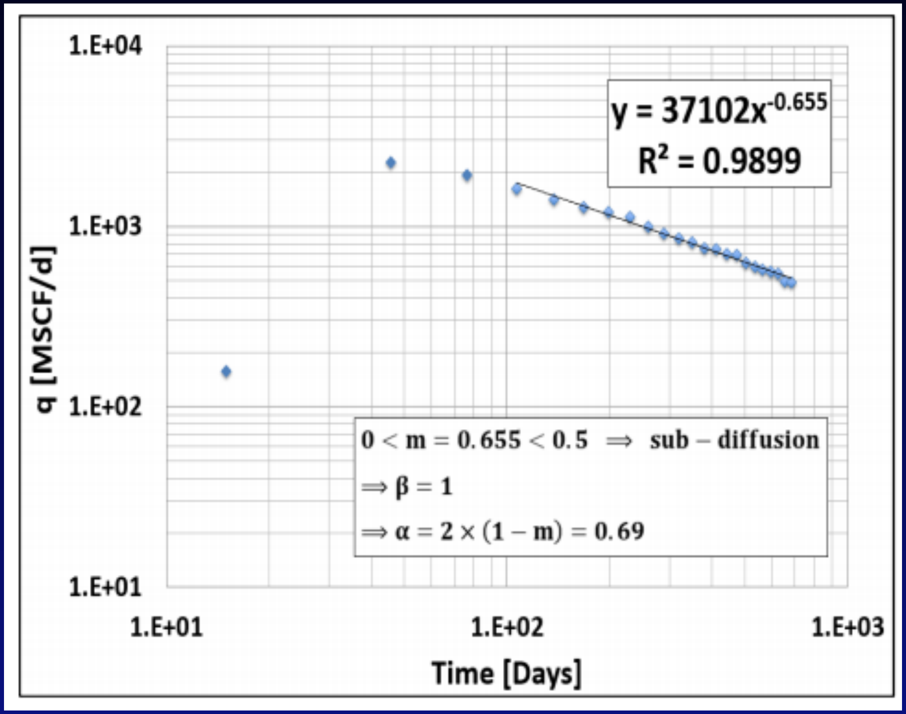
- As He et al. (2016) did, we will be simulating methane particles for the simplicity.
- Our main purpose is to calculate the $\frac{k_{\alpha\beta}}{\mu}$ parameter defined in Ralf's equation.
- Using the V, T and n, calculate the pressure of each node to calculate ΔP
- Δt: 10 femtoseconds
- For all the molecular simulation that we are planning to do, we will use LAMMPS
- Effect of temperature on the anomalous diffusion will be investigated

$$\frac{\partial}{\partial x}\frac{k_{\alpha\beta}}{\mu}\left(\frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\frac{\partial^{\beta} p(x,t)}{\partial x^{\beta}}\right) = (\phi c_t)_o \frac{\partial p(x,t)}{\partial t}$$

1-D anomalous diffusion – Field Application

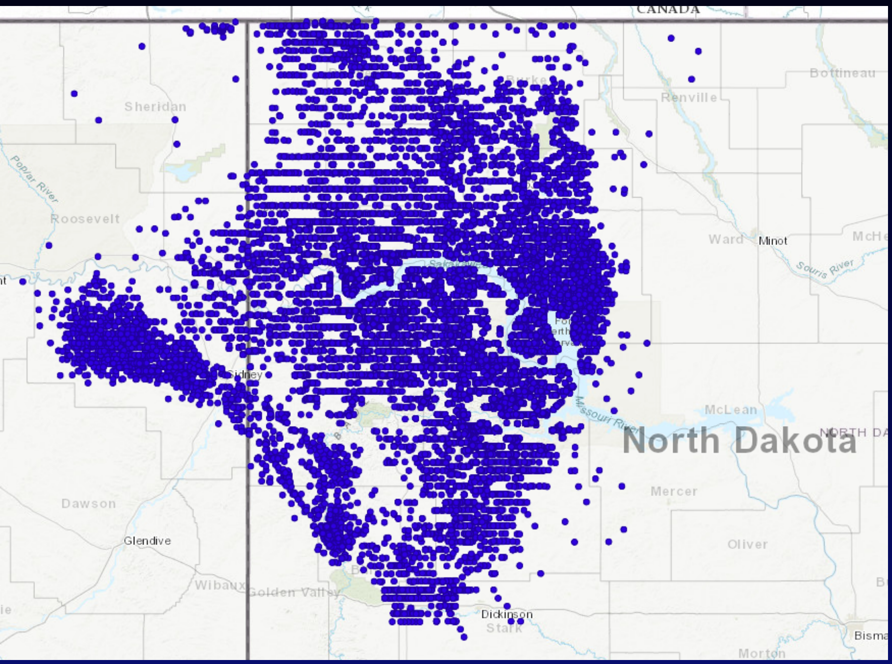


(API 42-497-36312)
Super diffusion in a Barnett gas well, Holy (2016)



(API 42-439-33141)
Sub diffusion in a Barnett gas well, Holy (2016)

Diffusion Types in an Unconventional Reservoir



Horizontal wells targeting Bakken and Three Forks, from Drillinginfo

- Monthly production data is available
- We will calculate the slope of the linear flow portion in each well
- The type of anomalous diffusion will be determined
    - Sub diffusion
    - Super diffusion
    - Normal diffusion
- Plot a heat map to see if there is a trend in the location of the wells and the type of diffusion as well as the slope of linear flow
- Investigate the relation between the slope from RTA, α from MSD vs time graph $(r^2 \sim t^{\wedge}\alpha)$ and the α and β parameters (spatial and time fractional derivative parameters)

Conclusion

- Initial findings in the literature
    - Kerogen creation, using kerogen to build a matrix system and simulating H.C.s in the matrix system
- Future plans
    - Extension of Ralf's 1-D anomalous diffusion model to 2-D
    - Investigating the anomalous diffusion parameters using a molecular dynamics model
- Analyzing the rate data of wells in a shale reservoir to investigate relationship between anomalous diffusion and location of the corresponding reservoir

References

Holy, R. W. & Ozkan, E. 2016. A practical and rigorous approach for production data analysis in unconventional wells, Presented at the SPE Low Perm Symposium, 5-6 May, Denver, Colorado, USA.

Kelemen, S. R.; Afeworki, M.; Gorbaty, M. L.; Sansone, M.; Kwiatek, P. J.; Walters, C. C.; Freund, H.; Siskin, M.; Bence, A. E.; Curry, D. J.; Solum, M.; Pugmire, R. J.; Vandenbroucke, M.; Leblond, M.; Behar, F. Direct Characterization of Kerogen by X-ray and SolidState 13C Nuclear Magnetic Resonance Methods. Energy Fuels 2007, 21 (3), 1548−1561

Nicolau, D. V., Jr, Hancock, J. F., & Burrage, K. (2006). Sources of anomalous diffusion on cell membranes: a Monte Carlo study. Biophysical journal, 92(6), 1975–1987. doi:10.1529/biophysj.105.076869

Ungerer, P., Collell, J., Yiannourakou, M., 2015. Molecular Modeling of the Volumetric and Thermodynamic Properties of Kerogen: Influence of Organic Type and Maturity. Energy & Fuels 29, 91–105. doi: 10.1021/ef502154k

Welch, W. R. W., & Piri, M. (2015, July 20). Molecular Dynamics Simulations of Retrograde Condensation in Nanoporous Shale. Unconventional Resources Technology Conference. doi:10.15530/URTEC-2015-2172738