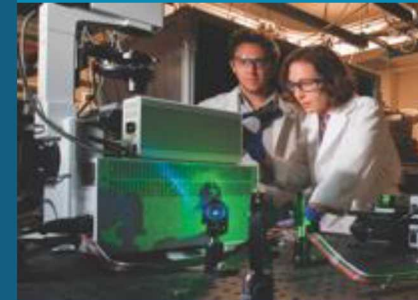




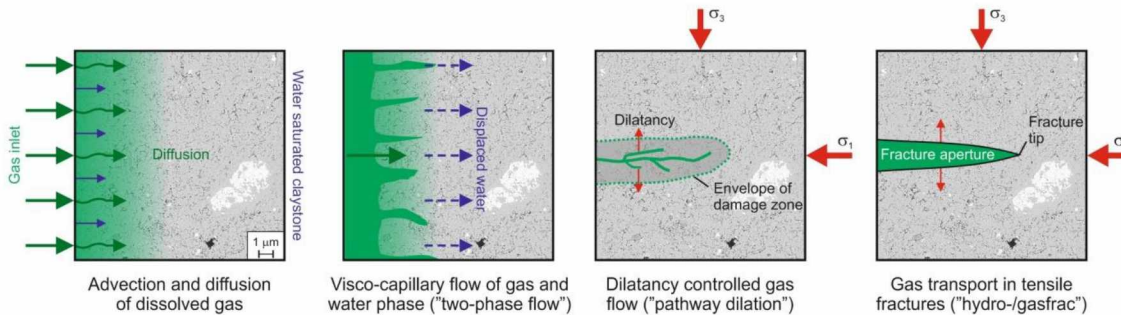
Sandia
National
Laboratories

SAND2018-11618PE

DECOVALEX19 TASK A: modElliNg Gas INjection ExpERiments (ENGINEER)



DECOVALEX19
WORKSHOP 6
Seoul, R. of Korea
Oct. 16-19, 2018



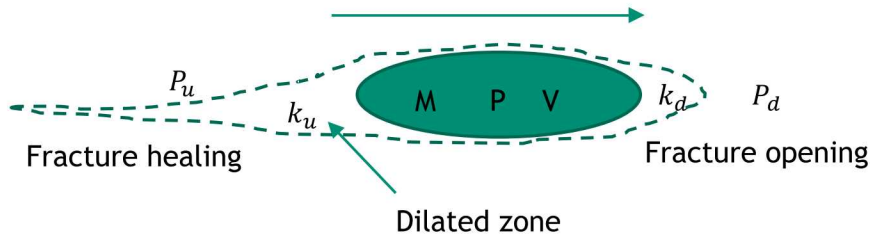
PRESENTED BY

Yifeng Wang (SNL), Boris Faybishenko (LBNL),
Jon Harrington (BGS)



Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525, SAND2018-3741 C

Bubble migration under a pressure gradient



Continuous logistic equation

$$\frac{dP}{dt} = \lambda_1 P \left(1 - \frac{P}{K}\right)$$

$$\lambda_1 = \frac{(k_u^0 P_u + k_d^0 P_d)RT}{V} \quad \lambda_2 = \frac{(k_u^0 + k_d^0)RT}{V} \quad K = \frac{\lambda_1}{\lambda_2}$$

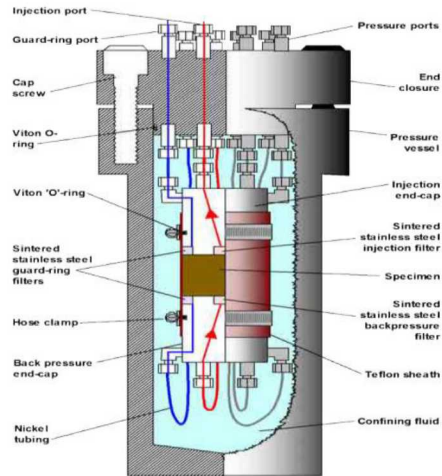
$$\frac{dM}{dt} = k_u(P_u - P) - k_d(P - P_d)$$

$$k_u = k_u^0 P \quad k_d = k_d^0 P \quad M = \frac{PV}{RT}$$

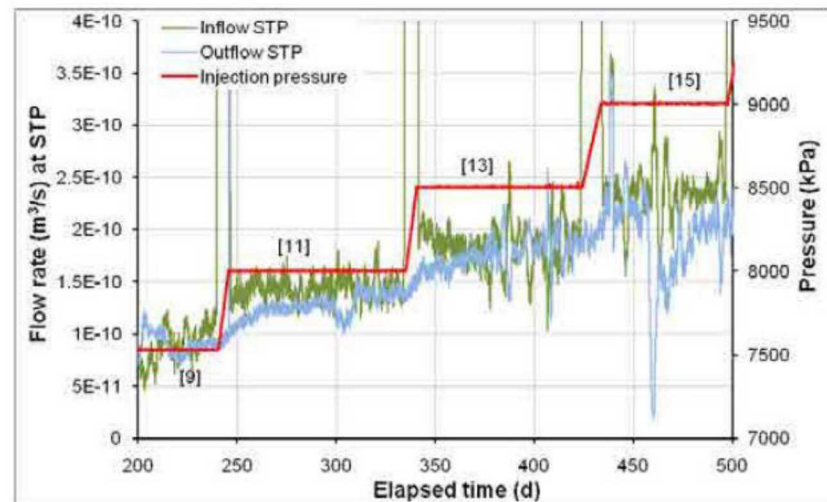
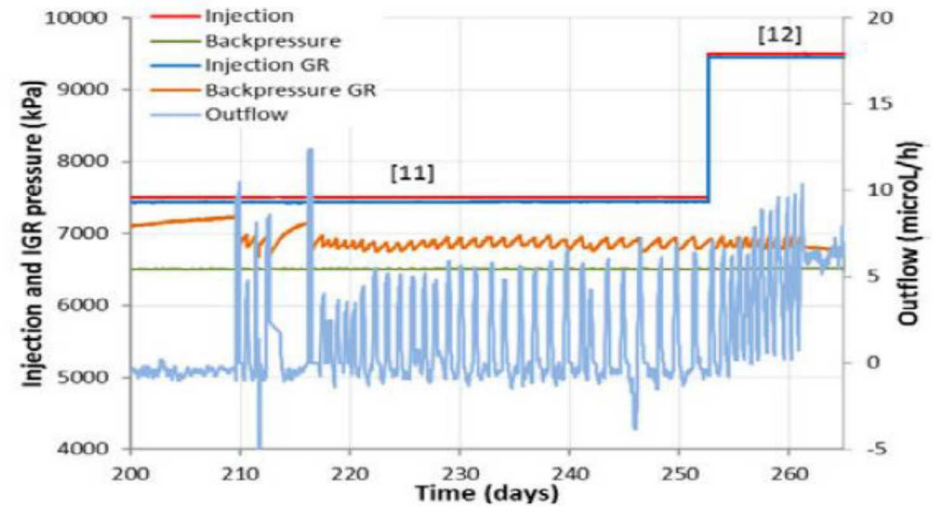
Delay logistic equation

$$\frac{dP}{dt} = \lambda_1 \left(1 - \frac{P}{K}\right) \int_{-\infty}^t G(t-s)p(s)ds$$

$$\frac{dP}{dt} = \lambda_1 \left(1 - \frac{P}{K}\right) \int_{-\infty}^t \alpha e^{-\alpha(t-s)} p(s)ds$$



FORGE Report D4.17 (Harrington, 2013)



Bubble migration under a pressure gradient: Chaotic behavior

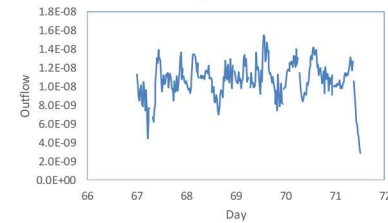
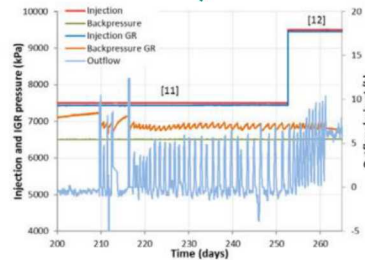
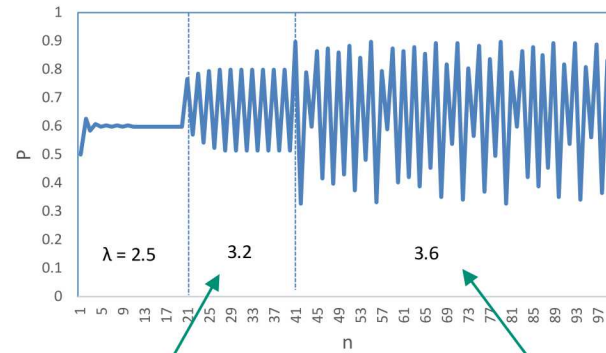


$$\frac{dP}{dt} = \lambda_1 p \left(1 - \frac{P}{K}\right)$$

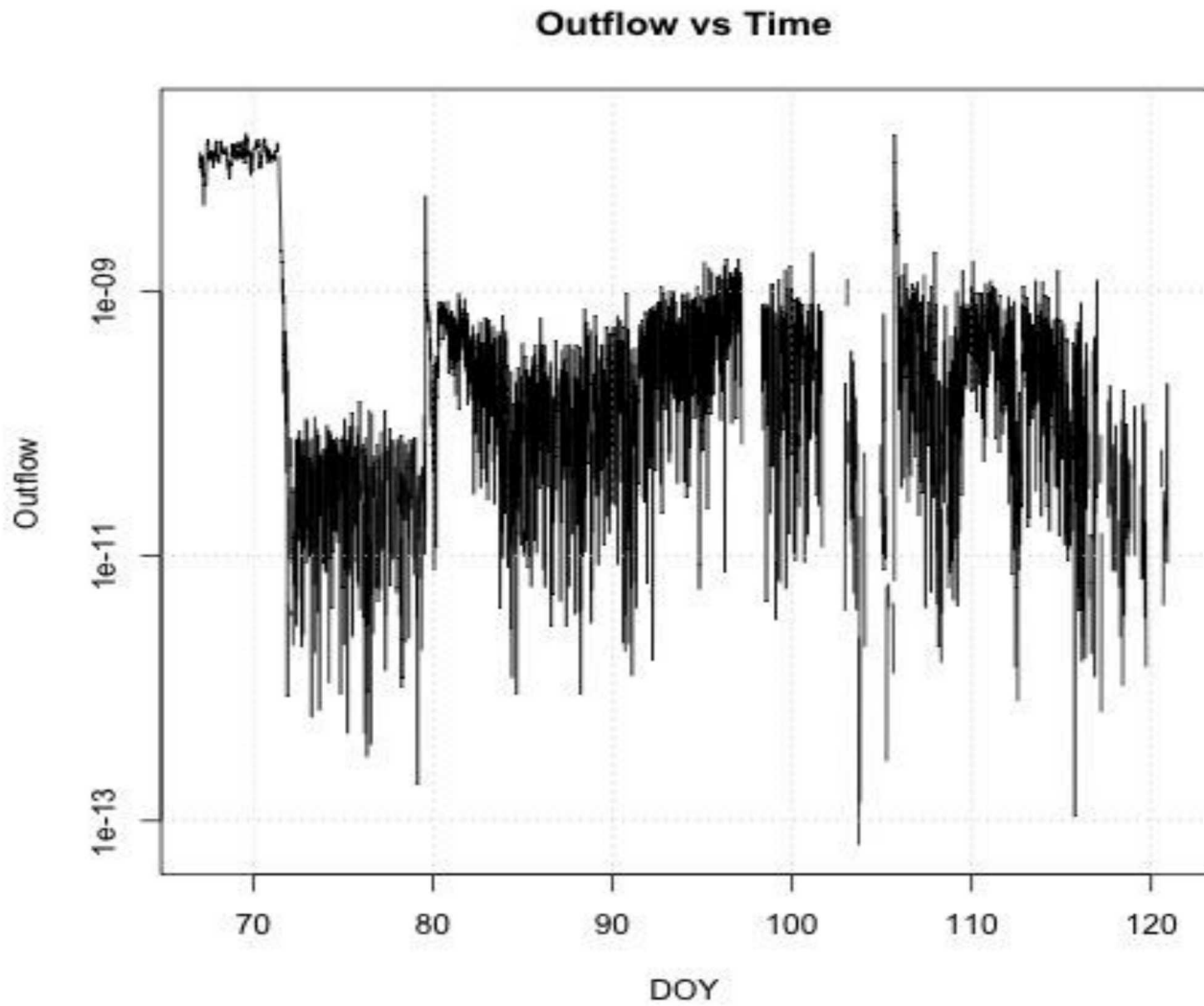
$$P_{n+1} = P_n + \lambda_1 P_n \left(1 - \frac{P}{K}\right) \Delta t$$

$$\lambda = 1 + \lambda_1 \Delta t$$

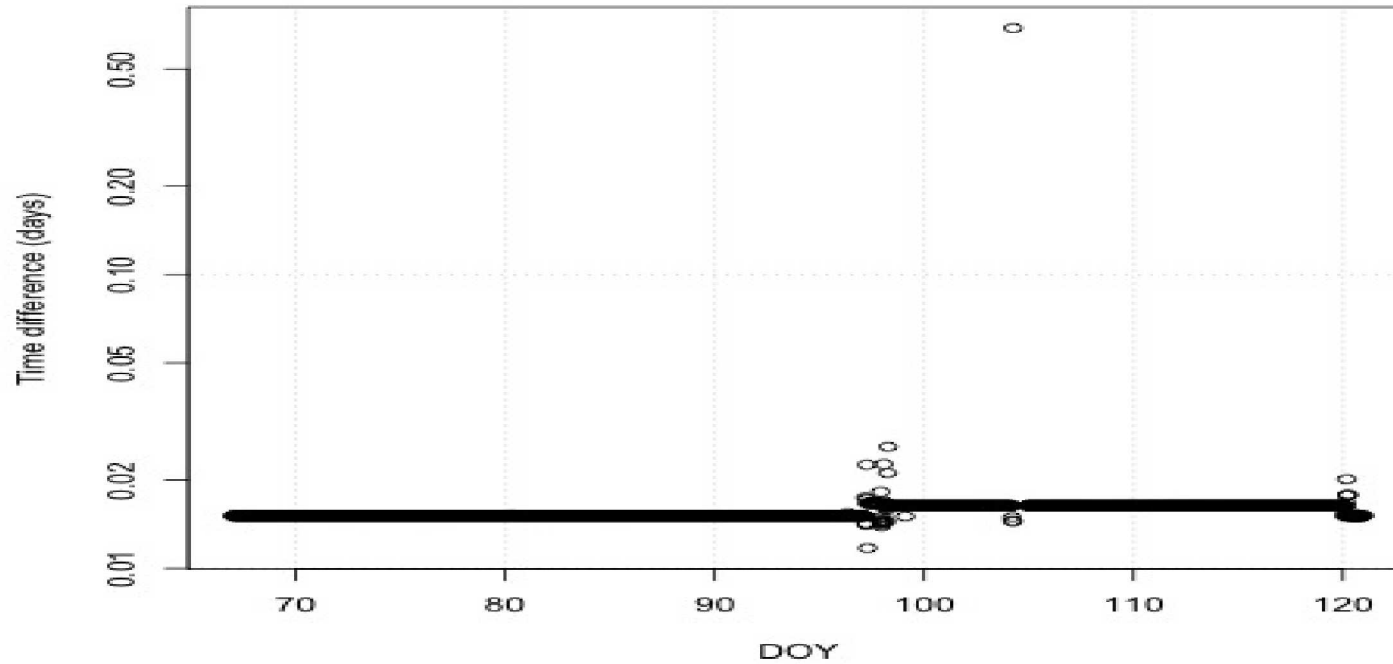
$$p_{n+1} = \lambda p_n (1 - p_n)$$



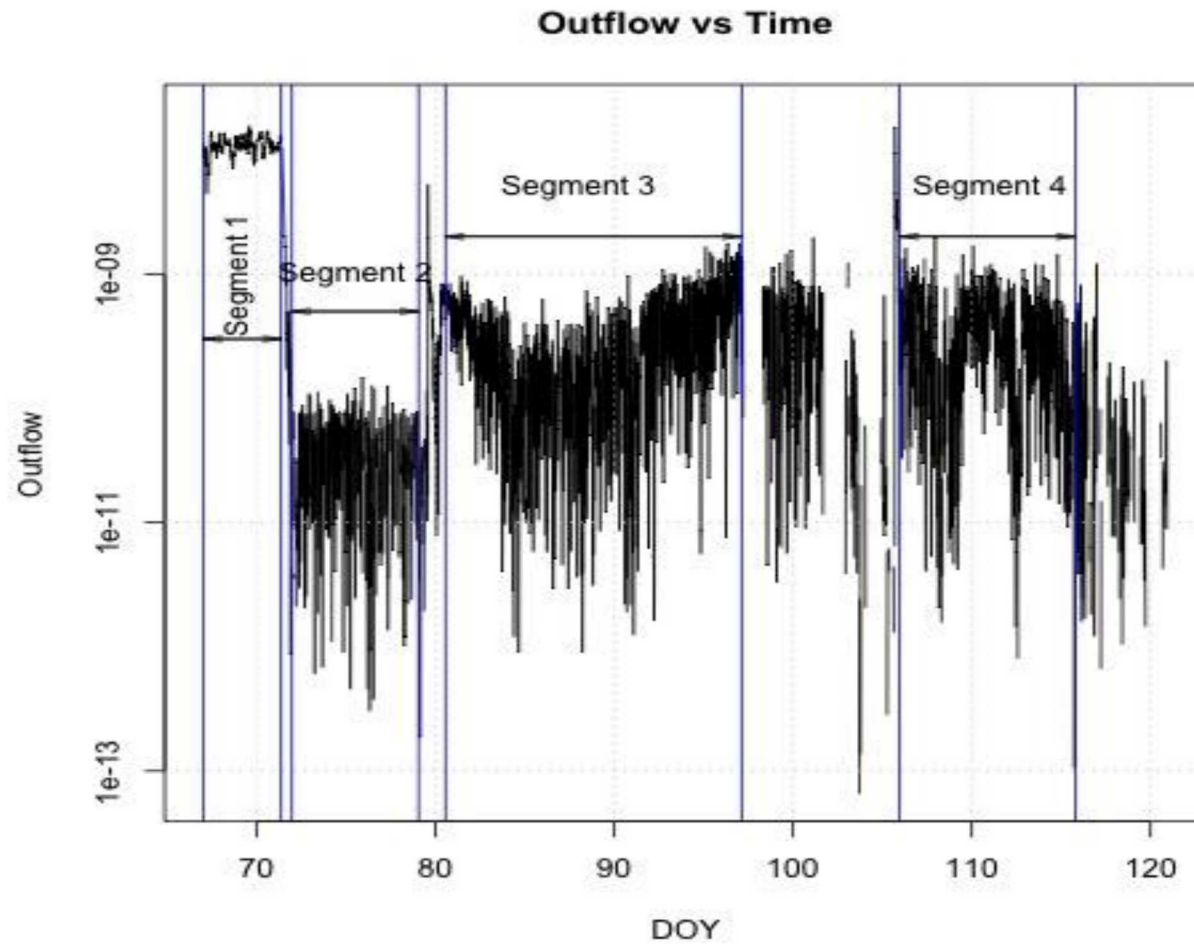
FORGE Report D4.17 (Harrington, 2013)



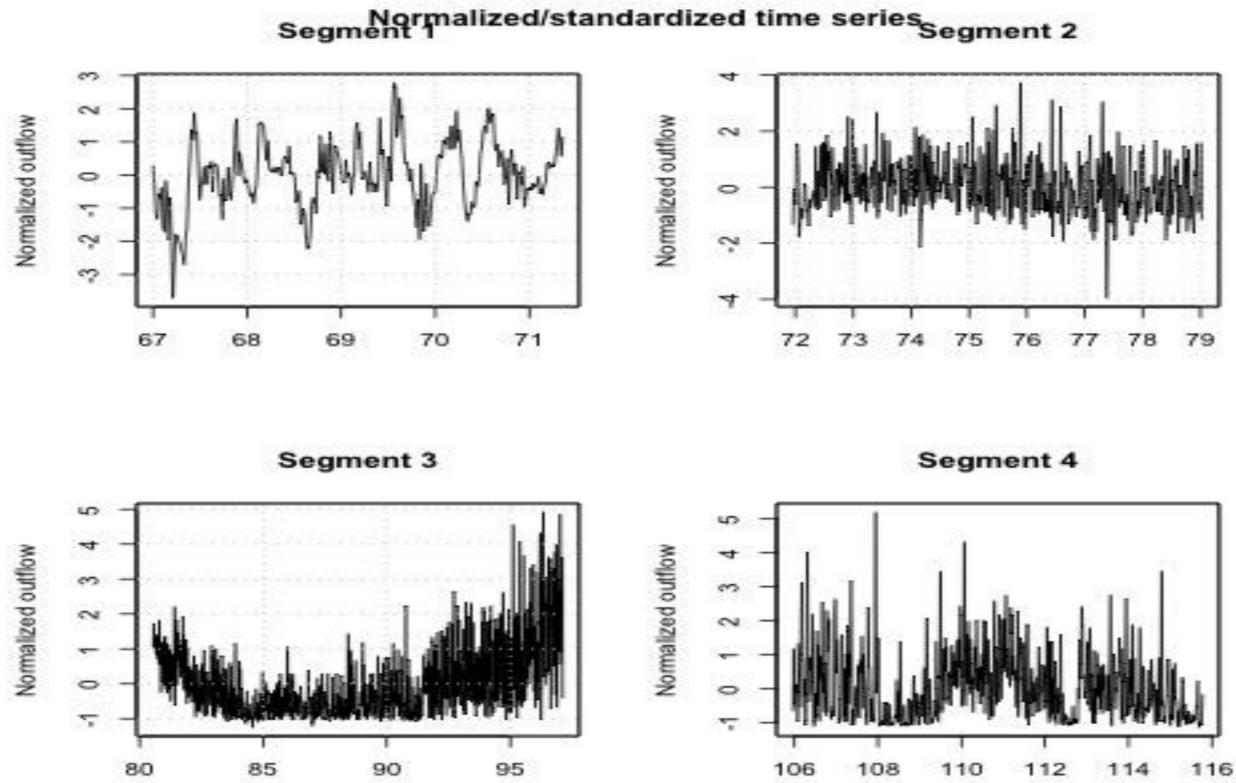
Time series of the time difference between measurements



Segmentation of the time series: 4 segments are defined



Normalized time series plots



Time series were scaled/ standardized by subtracting the mean and dividing by the standard deviation.



The additive model used is:

$$Y[t] = \text{Trend}[t] + \text{Periodic}[t] + \text{Stochastic}[t]$$

The multiplicative model used is:

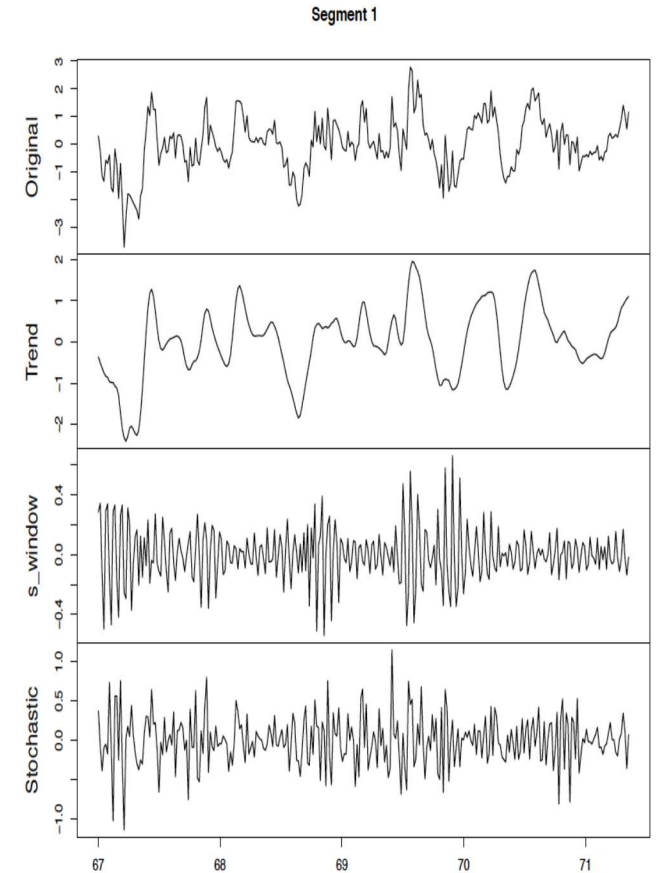
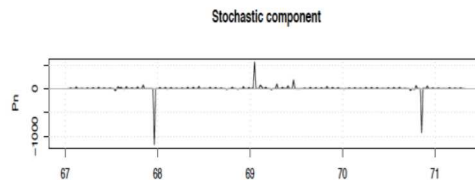
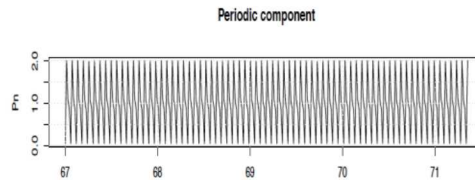
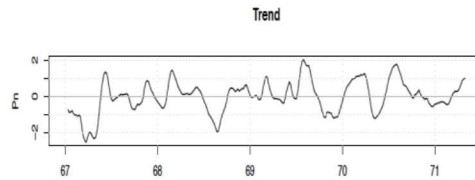
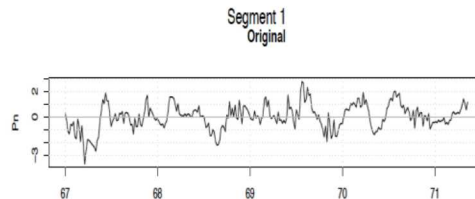
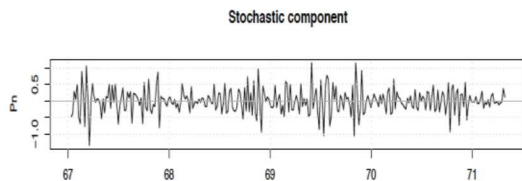
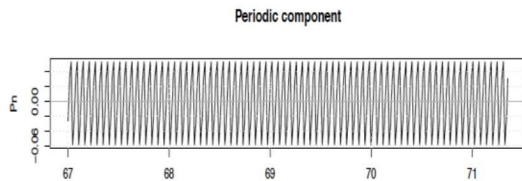
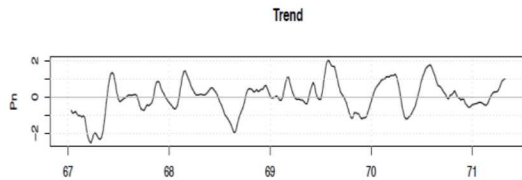
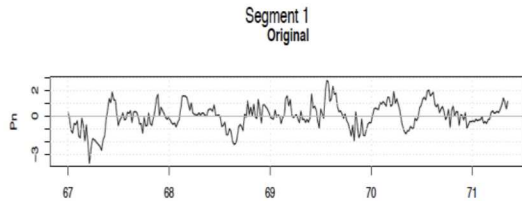
$$Y[t] = \text{Trend}[t] * \text{Periodic}[t] * \text{Stochastic}[t]$$

STL Model (Polynomial regression--variation of the additive model)

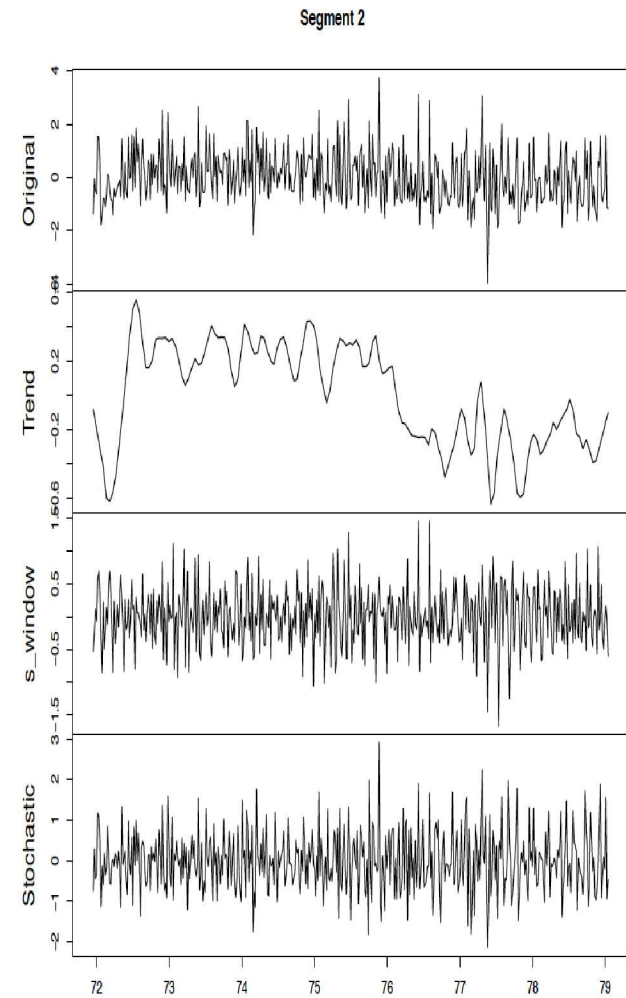
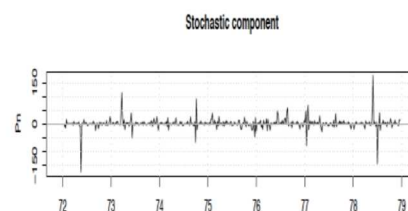
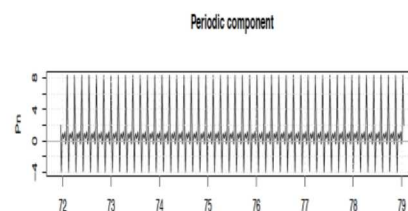
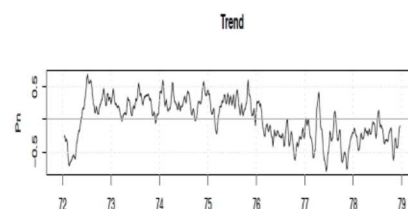
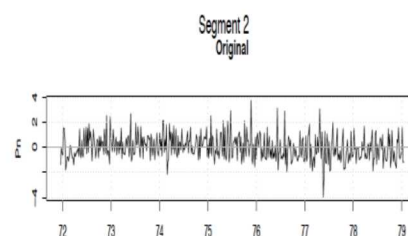
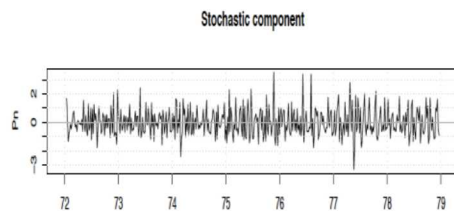
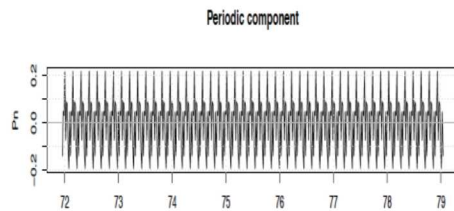
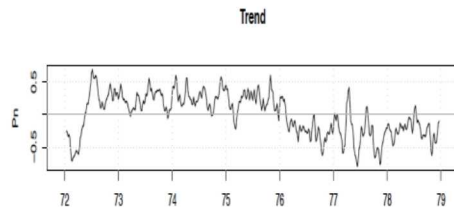
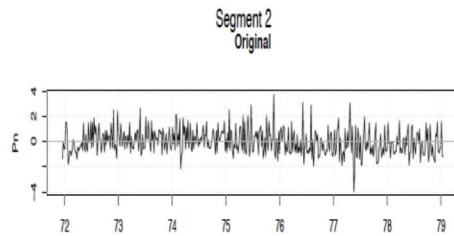
There are three components of a time series:

- trend of the overall changing
- Periodic component
- Stochastic -- error/residual/irregular component not explained by the trend or the periodic value

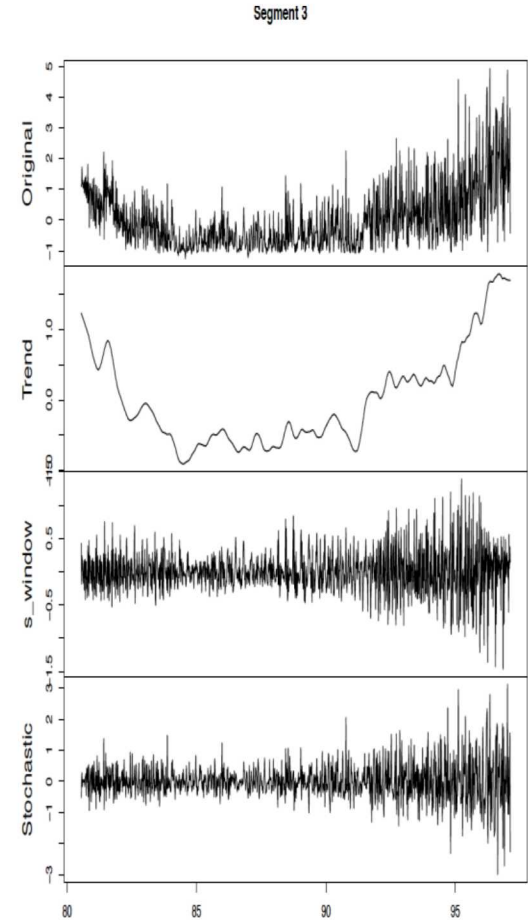
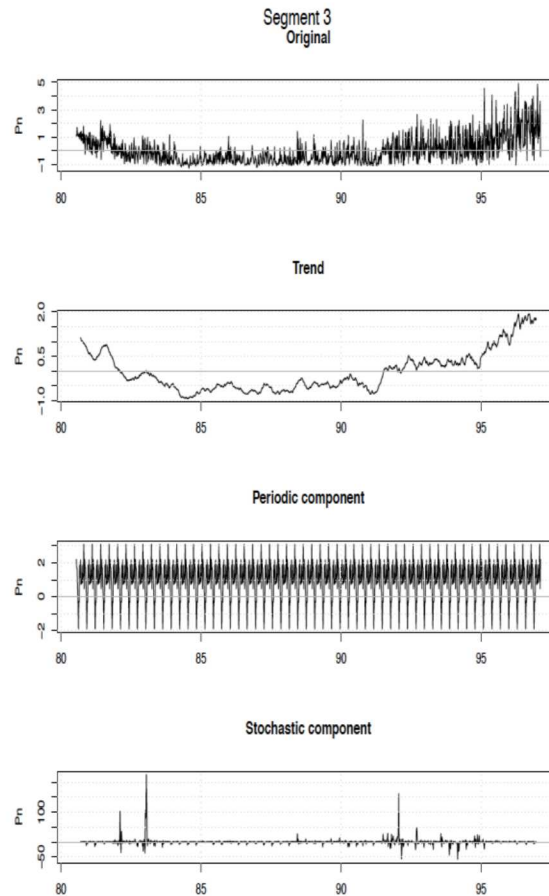
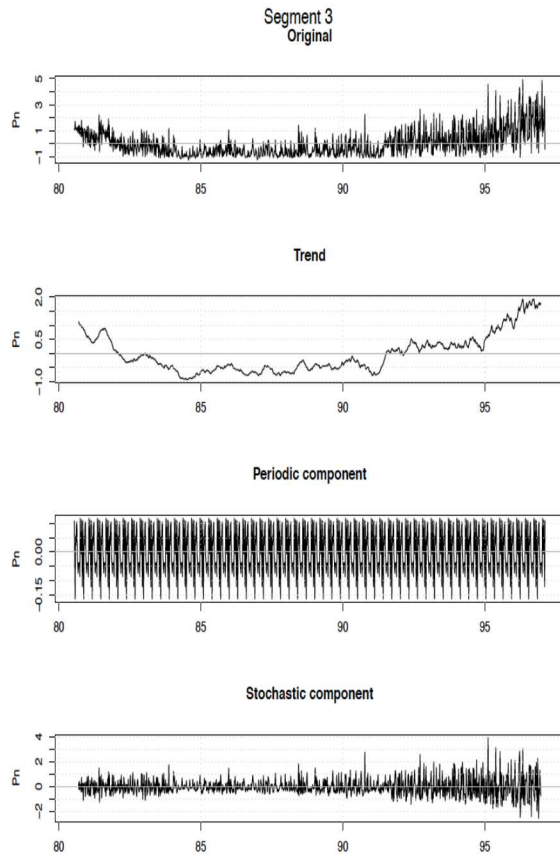
Graphical Comparison of Decomposition Models: Segment I



Graphical Comparison of Decomposition Models: Segment 2



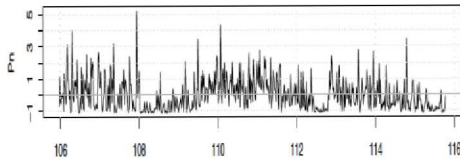
Graphical Comparison of Decomposition Models: Segment 3



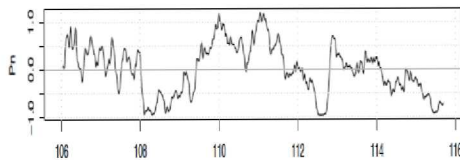
Graphical Comparison of Decomposition Models: Segment 4



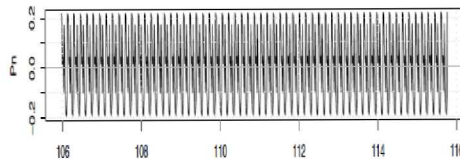
Segment 4
Original



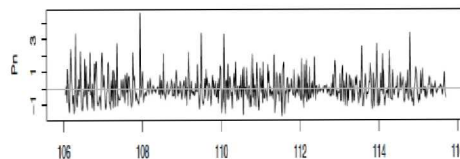
Trend



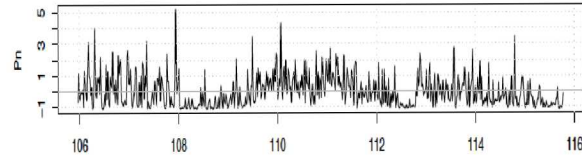
Periodic component



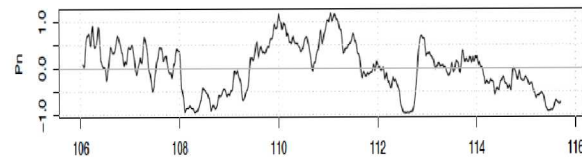
Stochastic component



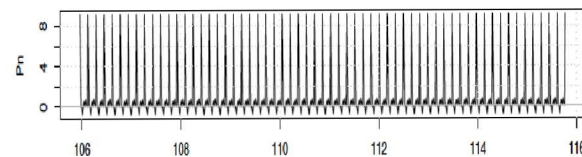
Segment 4
Original



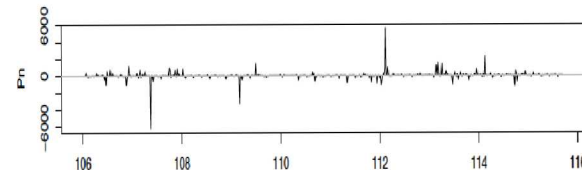
Trend



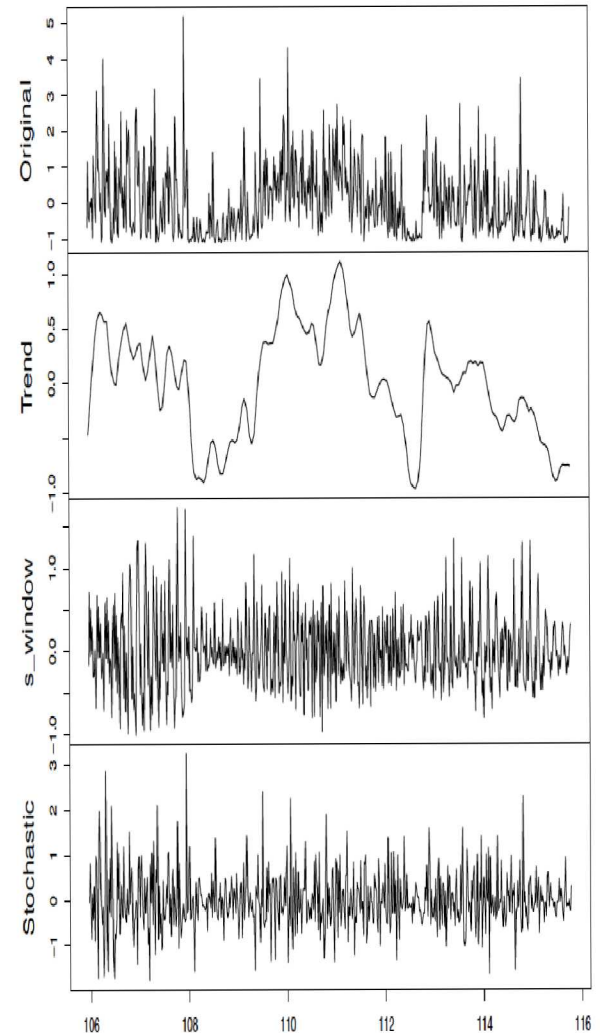
Periodic component



Stochastic component



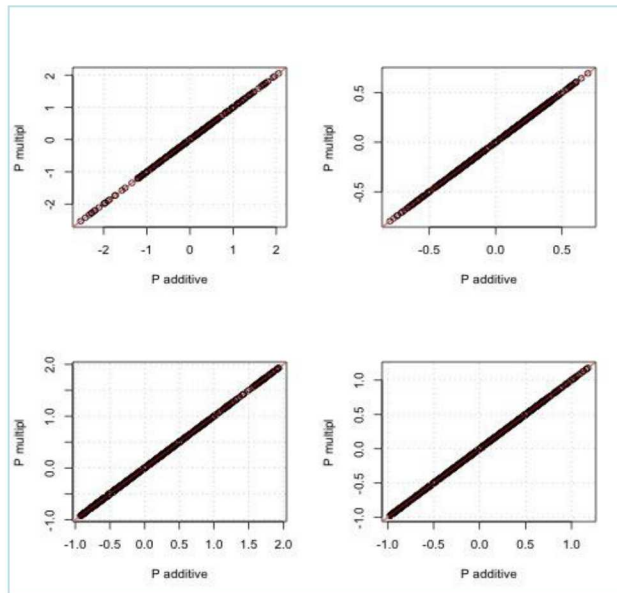
Segment 4



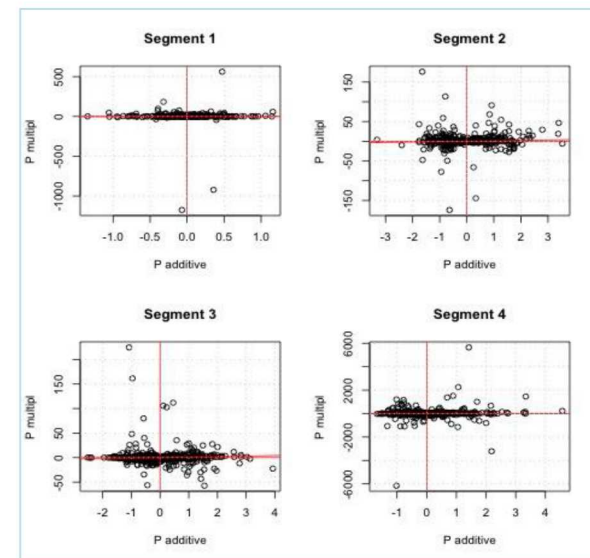
Comparison of Decompositions



1:1 correlations between the trends determined using different types of decomposition

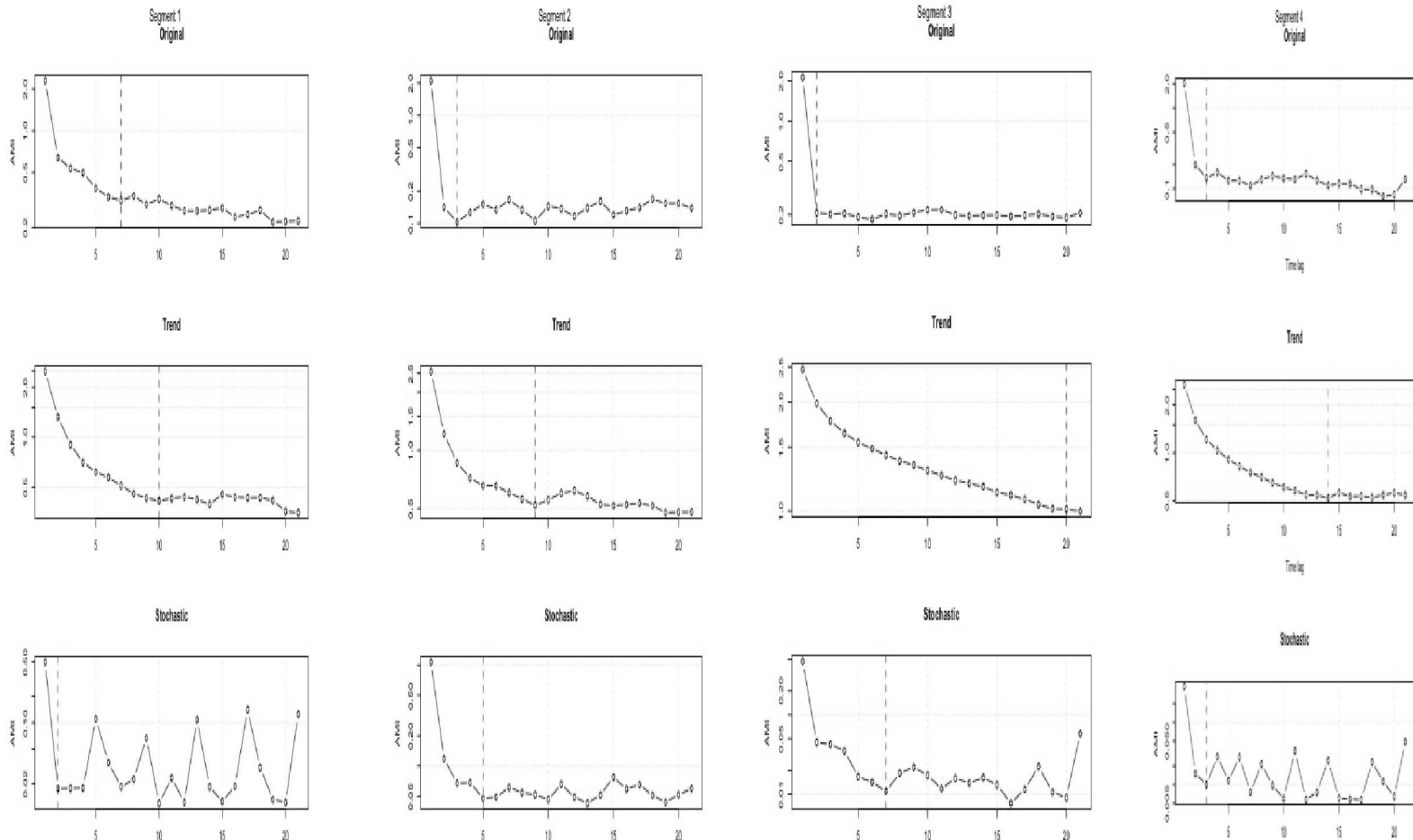


Minimal stochastic component is determined using the multiplicative decomposition



An application of the Autocorrelation Function (ACF) shows that the measured time series is a **MULTIPLICATIVE FUNCTION**, which is typical for the nonlinear dynamics

Time lags calculated for the original, trend, and stochastic components from multiplicative decomposition

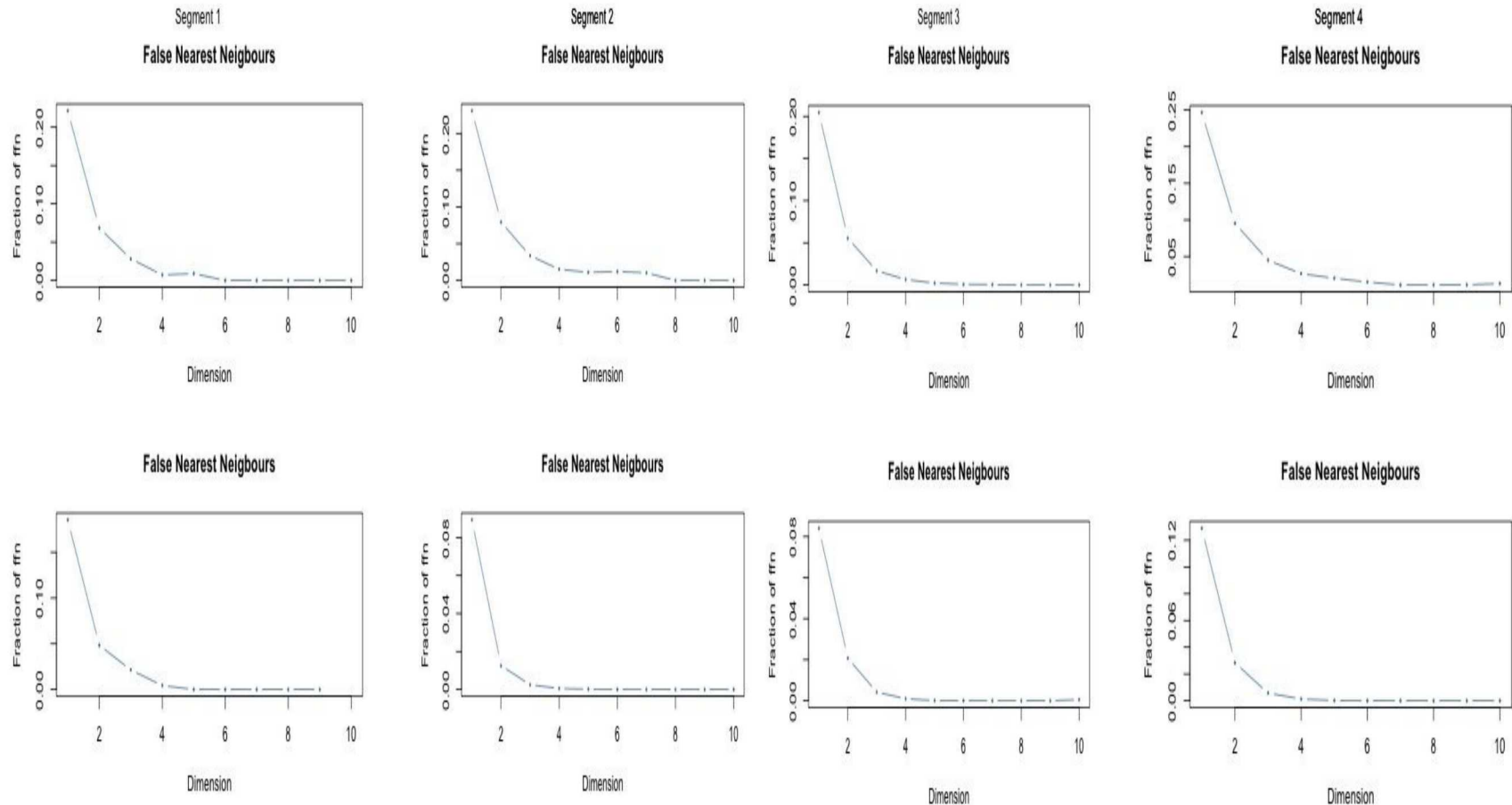


- Calculated from the 1st minimum of the average mutual information function
 - Vertical lines - time lags

Time lags (time delays) of multiplicative decomposition components of the original, trend, and stochastic components of time series, which were used for calculations of diagnostic parameters of deterministic chaos and plotting the pseudo-phase attractors

	Segment 1	Segment 2	Segment 3	Segment 4
Original	7	3	2	3
Trend	10	9	20	14
Stochastic	2	5	7	3

Global Embedding Dimension calculated using the False Nearest Neighbors Method

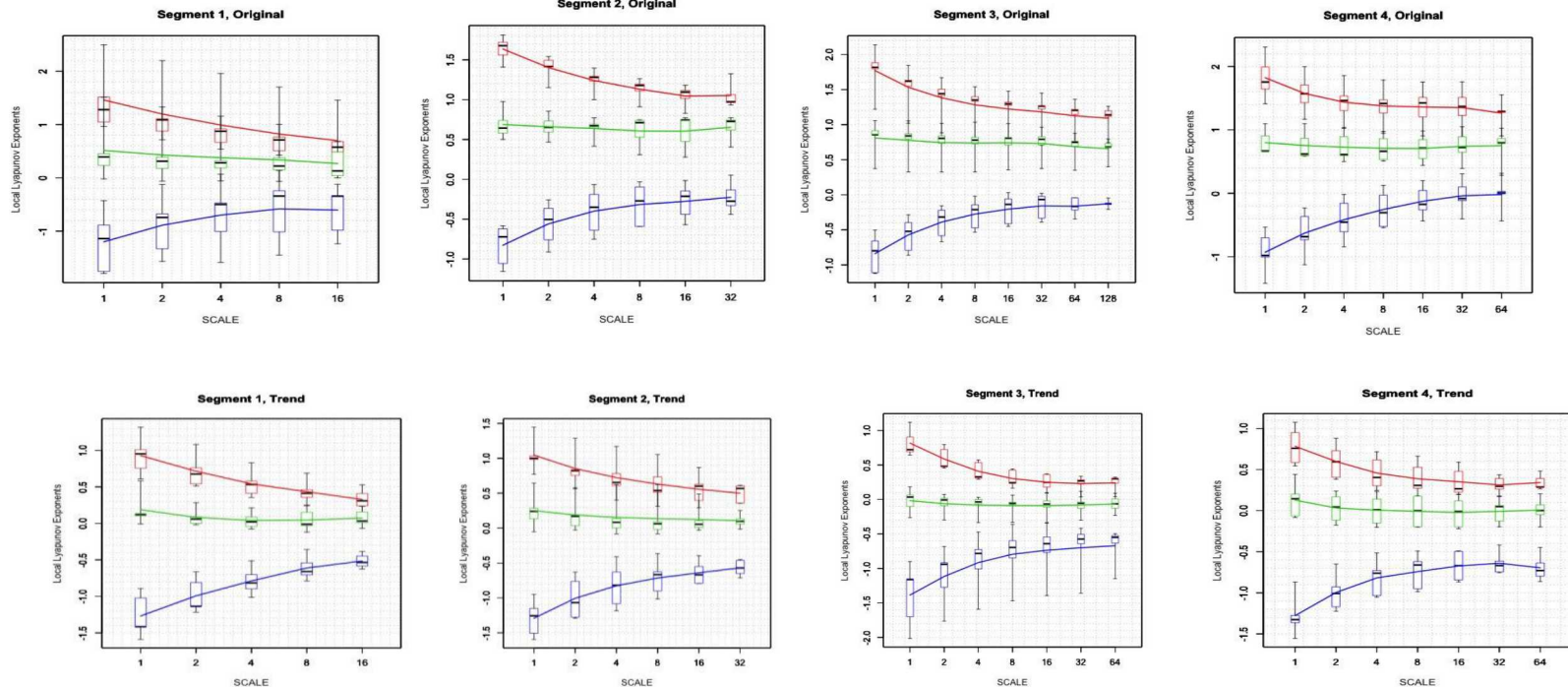


Embedding dimension of all time series trends is 4, which is a diagnostic feature of low-dimensional chaos.

Calculations of the spectrum of 3 Local exponents Lyapunov



No zero Lyap exp for original data - there is a random component



All time series contain a positive Lyapunov exponents, which is a typical feature of deterministic chaos.

Trends have 1 exponents ~ 0 , and the sum of Lyapunov exponents is < 0 , which are typical features of deterministic chaos. (Calculations will be performed with 4 Local Lyapunov exponents).

Correlation integral (at multiple length scales)

	Original	Trend	Stoch
Segment 1	2.123	2.104	2.466
Segment 2	2.132	2.044	2.360
Segment 3	2.120	2.078	2.346
Segment 4	2.121	2.063	2.601

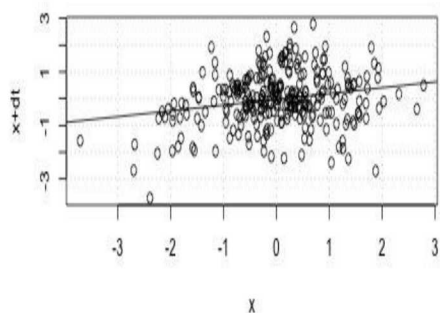
Correlation dimension and information dimension

	Intr_dim	Local_Inf_dim_1	Cor_dim	Local_Inf_dim_2
Segment 1	8.436 (?)	1.821	1.922	1.913
Segment 2	2.226	2.177	1.719	1.486
Segment 3	2.042	1.943	1.932	1.907
Segment 4	2.256	1.520	1.719	1.404

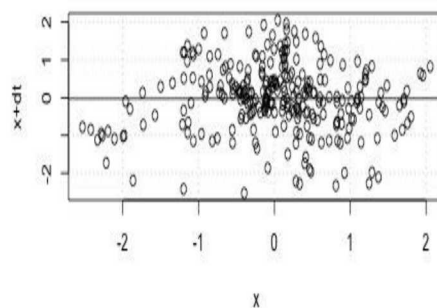
All diagnostic parameters indicate that all time series data are deterministic chaotic.



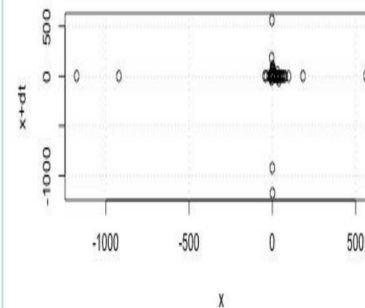
2D attractor, Segment 1, Original



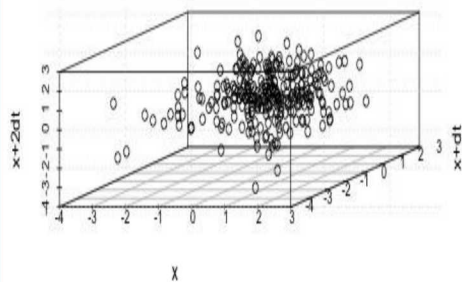
2D attractor, Segment 1, Trend



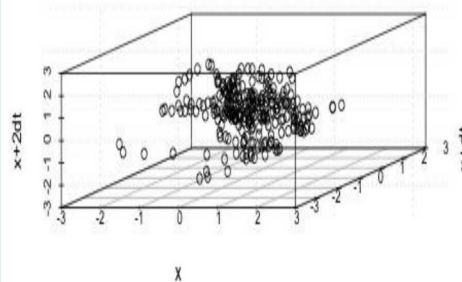
2D attractor, Segment 1, Stochastic



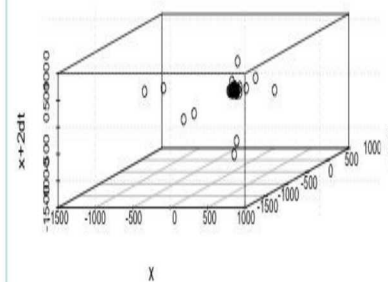
3D attractor, Segment 1, Original



3D attractor, Segment 1, Trend



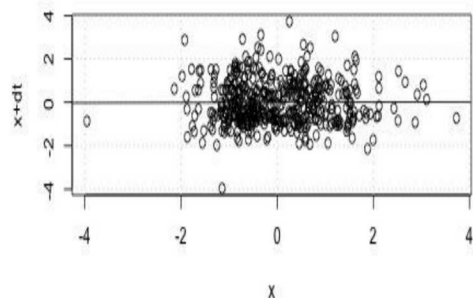
3D attractor, Segment 1, Stochastic



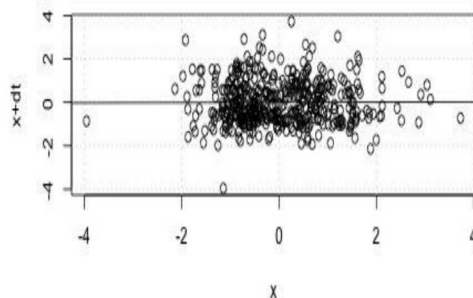
Attractors are plotted using time lags Δt shown above on the figures and in the table



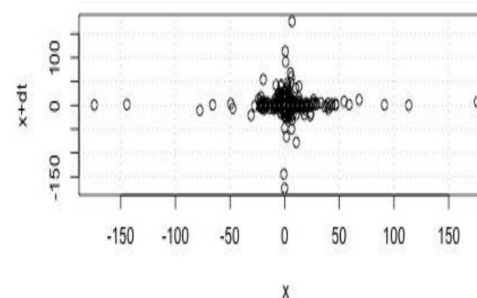
2D attractor, Segment 2, Original



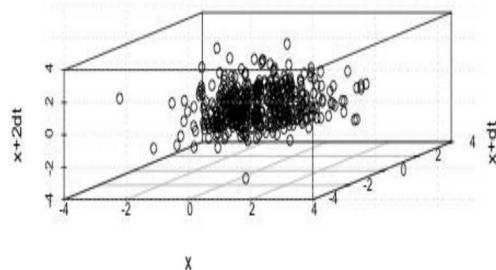
2D attractor, Segment 2, Trend



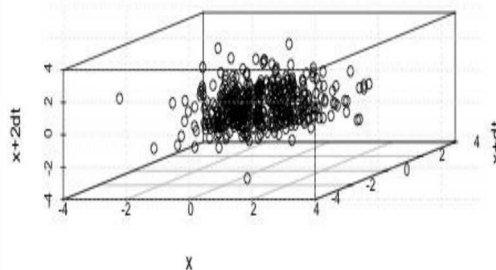
2D attractor, Segment 2, Stochastic



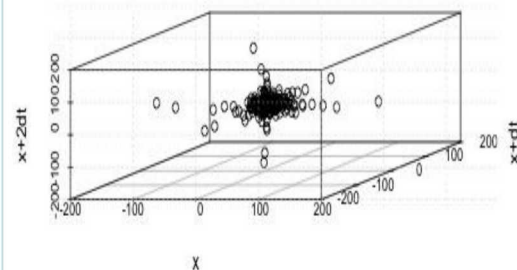
3D attractor, Segment 2, Original



3D attractor, Segment 2, Trend

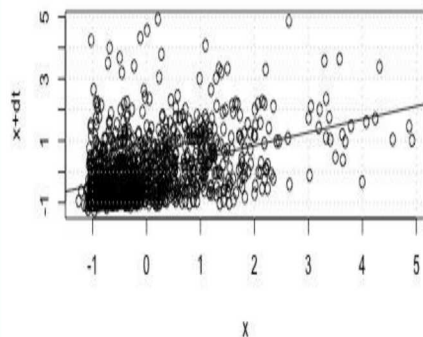


3D attractor, Segment 2, Stochastic

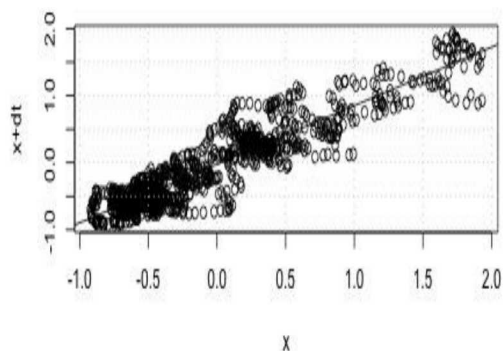




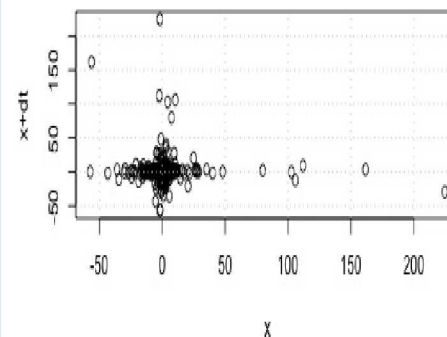
2D attractor, Segment 3, Original



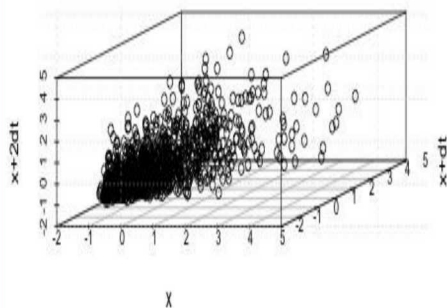
2D attractor, Segment 3, Trend



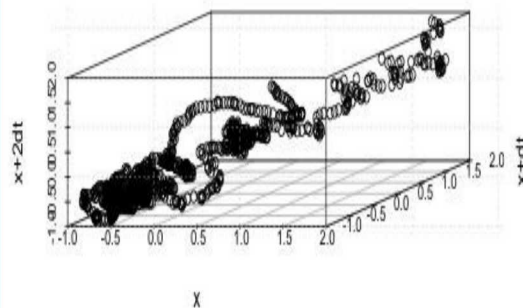
2D attractor, Segment 3, Stochastic



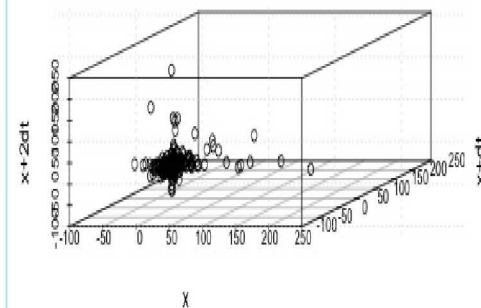
3D attractor, Segment 3, Original



3D attractor, Segment 3, Trend

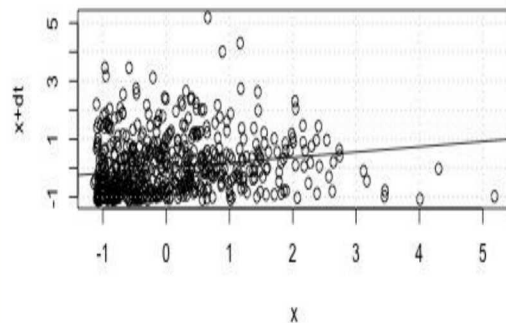


3D attractor, Segment 3, Stochastic

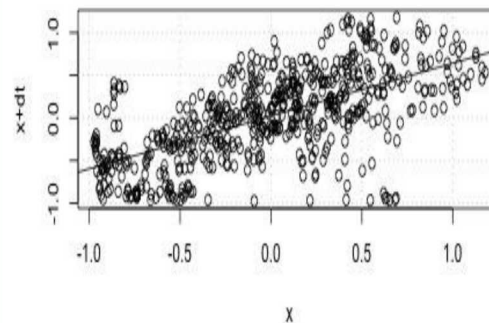




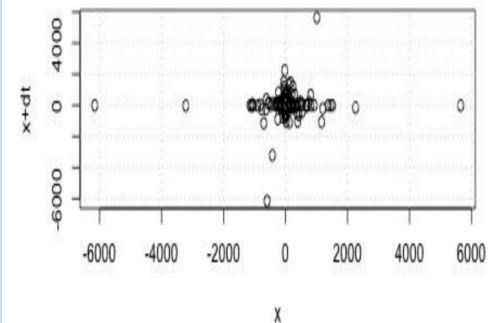
2D attractor, Segment 4, Original



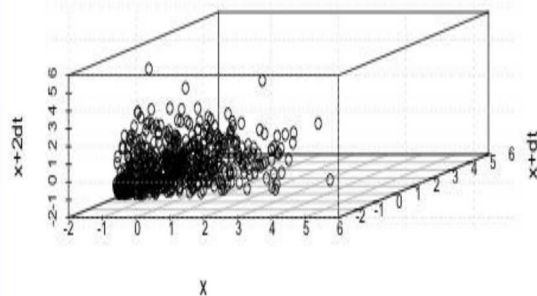
2D attractor, Segment 4, Trend



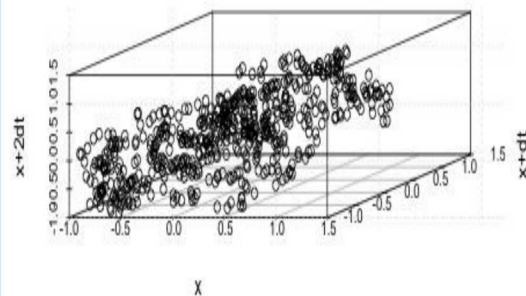
2D attractor, Segment 4, Stochastic



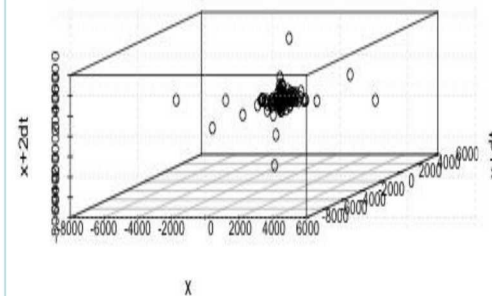
3D attractor, Segment 4, Original



3D attractor, Segment 4, Trend



3D attractor, Segment 4, Stochastic



Concluding remarks



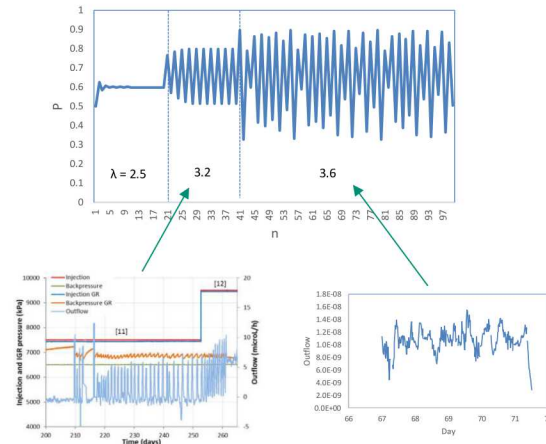
- The outflow data collected during the gas injection experiment show that gas migration in the system is deterministically chaotic.
- The dimension of the nonlinear dynamic system is ~ 3 to 4.
- Next steps:
 - Prepare and submit a peer-reviewed paper.
 - Develop a set of ODEs (or PDEs) of equations) to describe chaotic gas migration behaviors.
 - Use experimental data for model validation and verification.

$$\frac{dP}{dt} = \lambda_1 p \left(1 - \frac{P}{K}\right)$$

$$P_{n+1} = P_n + \lambda_1 P_n \left(1 - \frac{P}{K}\right) \Delta t$$

$$\lambda = 1 + \lambda_1 \Delta t$$

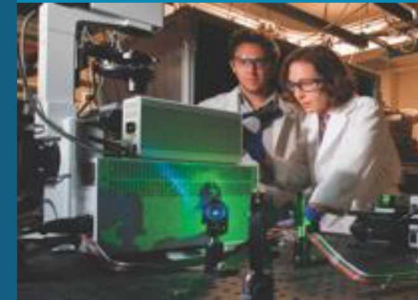
$$p_{n+1} = \lambda p_n (1 - p_n)$$



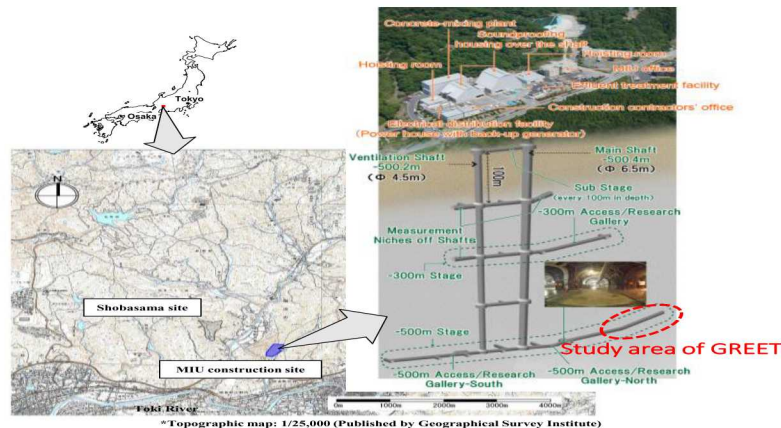


Sandia
National
Laboratories

DECOVALEX19 TASK C: GREET Step 2b Hydrology Analysis Update



DECOVALEX19
WORKSHOP 6
Seoul, R. of Korea
Oct. 16-19, 2018



PRESENTED BY

Yifeng Wang, Teklu Hadgu, Elena Kalinina



Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525, SAND2018-3741 C

Task C: Update on Hydrology Analysis



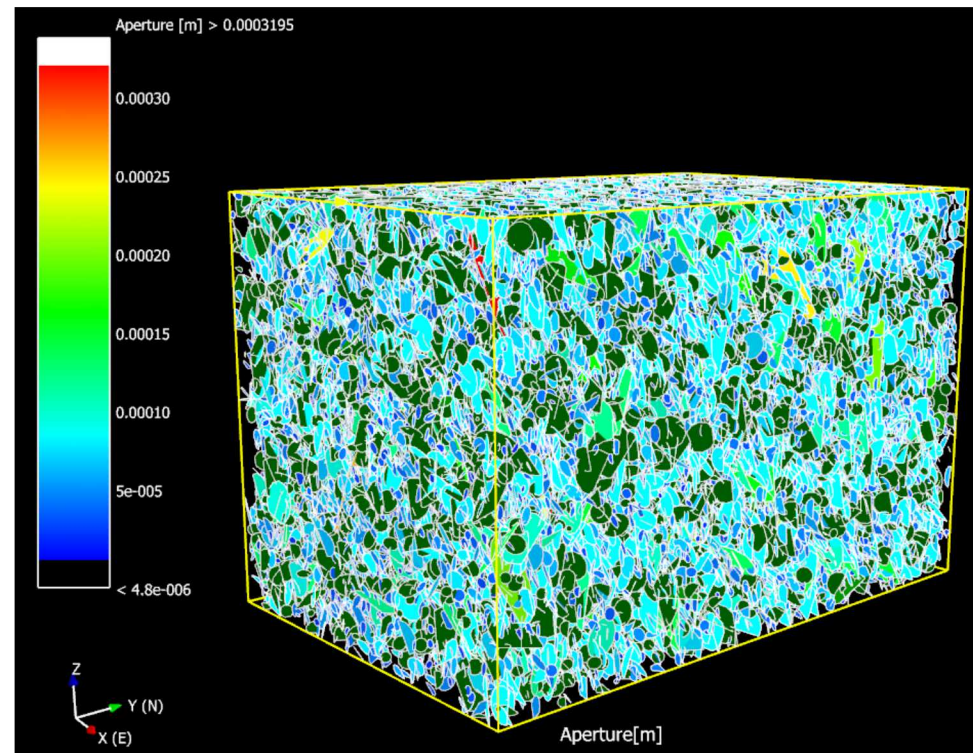
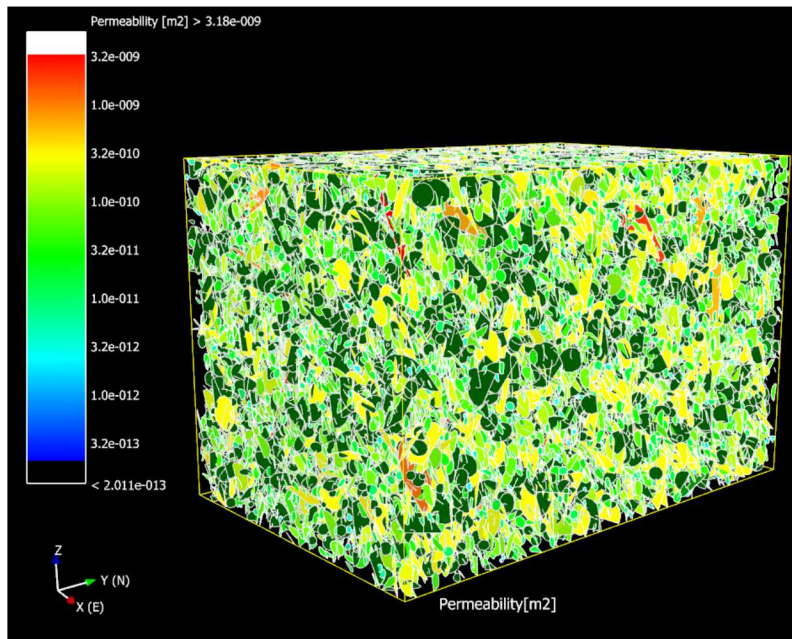
- Step 2b – Updated flow modeling of CTD filling and recovery.
- Used previously generated modeling tools.
- Conducted calibration analysis to match experimental data in CTD and observation points in borehole 12MI33.

Step2b Pressure Recovery Model Setup

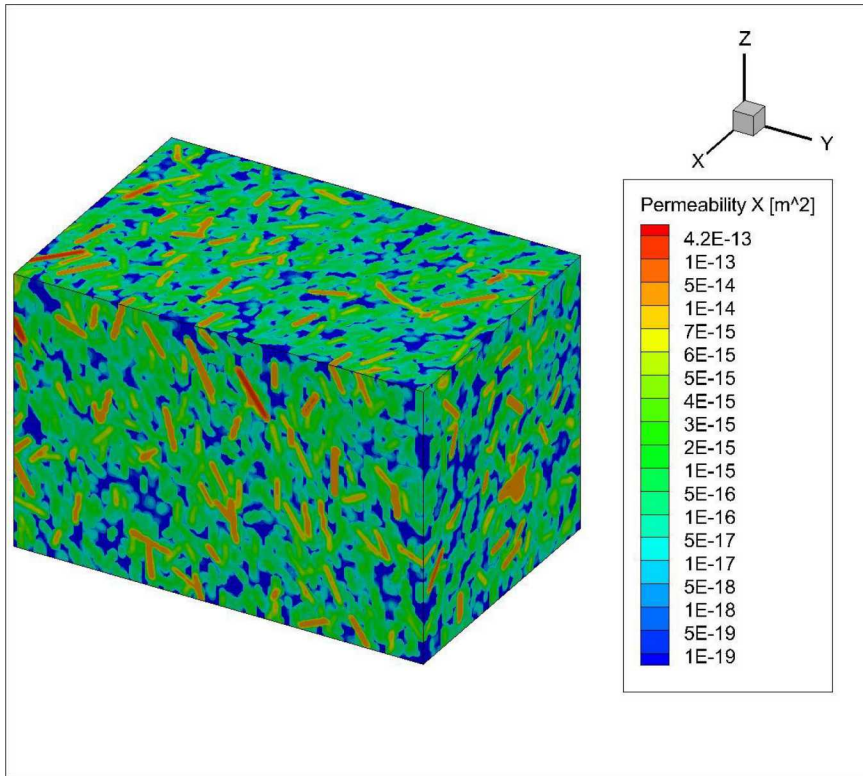


- Domain: 200 m x 300 m x 200 m.
- Grid block size: 2 m x 2 m x 2m.
- Mesh Size: 1,500,000 grid blocks.
- Fracture model with two fracture sets.
 - Realization 2 selected.
 - Permeability and porosity upscaled to continuum grid.
- Analysis also includes using Realization 9 and a Homogenous system ($k = 10^{-15} \text{ m}^2$)
- PFLOTRAN numerical code was used for flow simulations.

Step2b: DFN Data for Realization 2

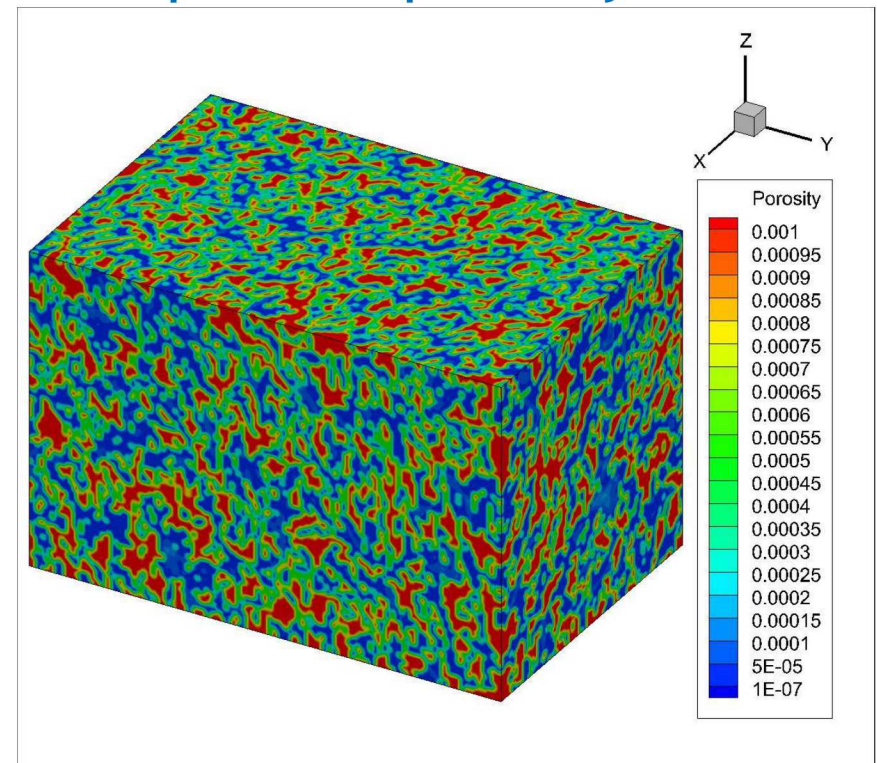


Step2b: Upscaled Permeability and Porosity Fields for Realization 2

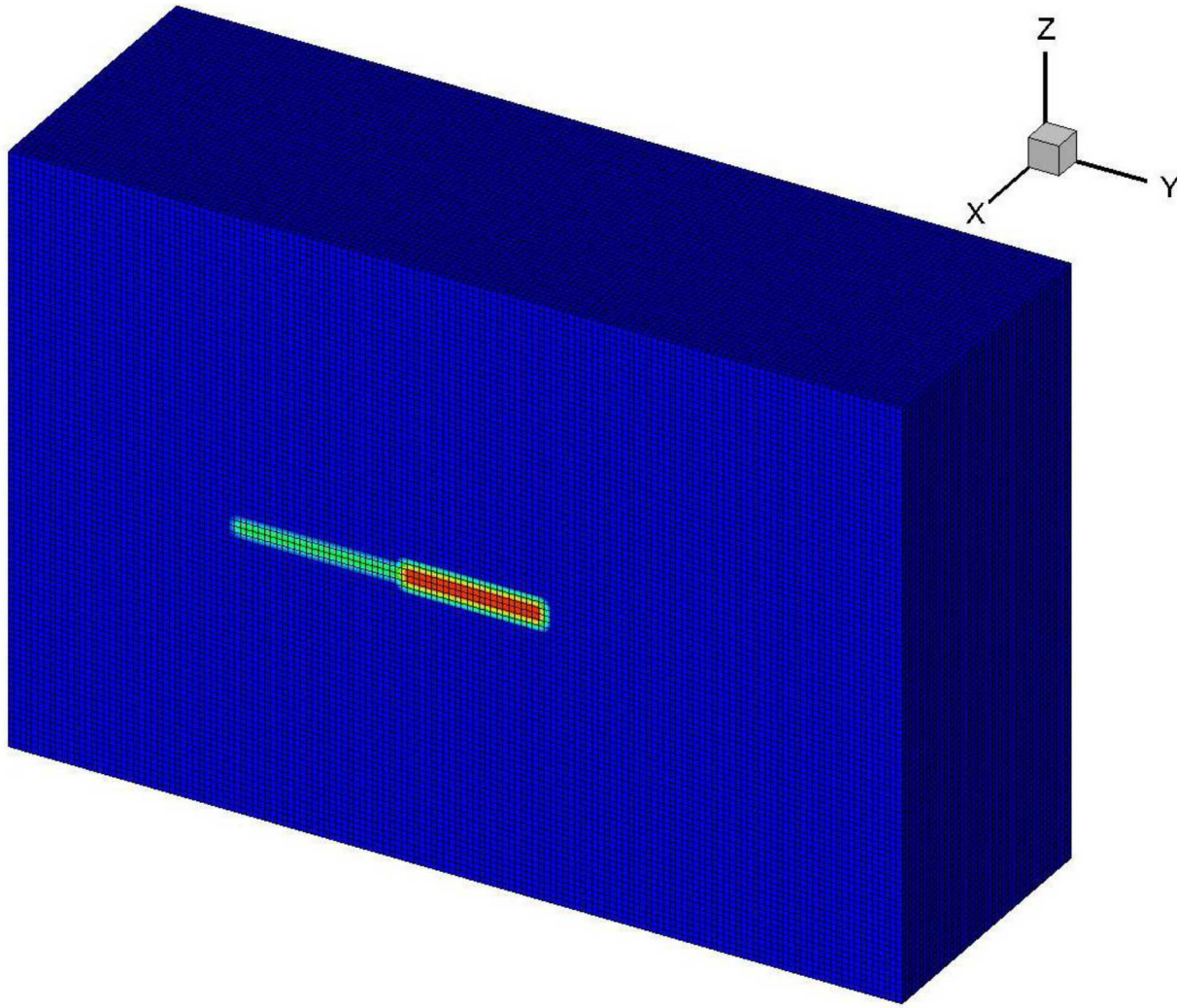


Upscaled permeability field

Upscaled porosity field



Step2b: Location of Inclined Drift and CTD



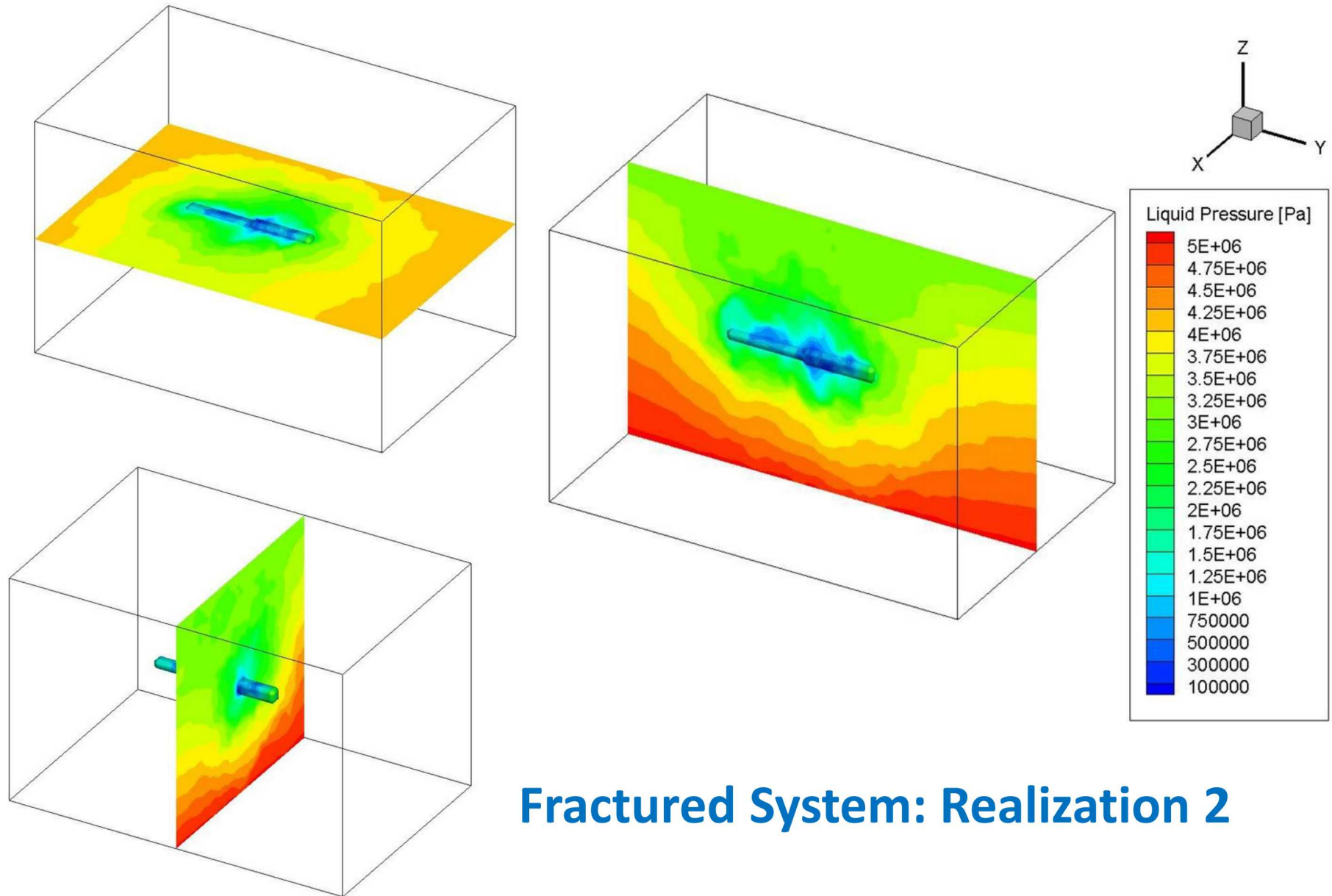
Location of Inclined Drift and CTD in domain

Part I - Step 2b Updated Flow Modeling

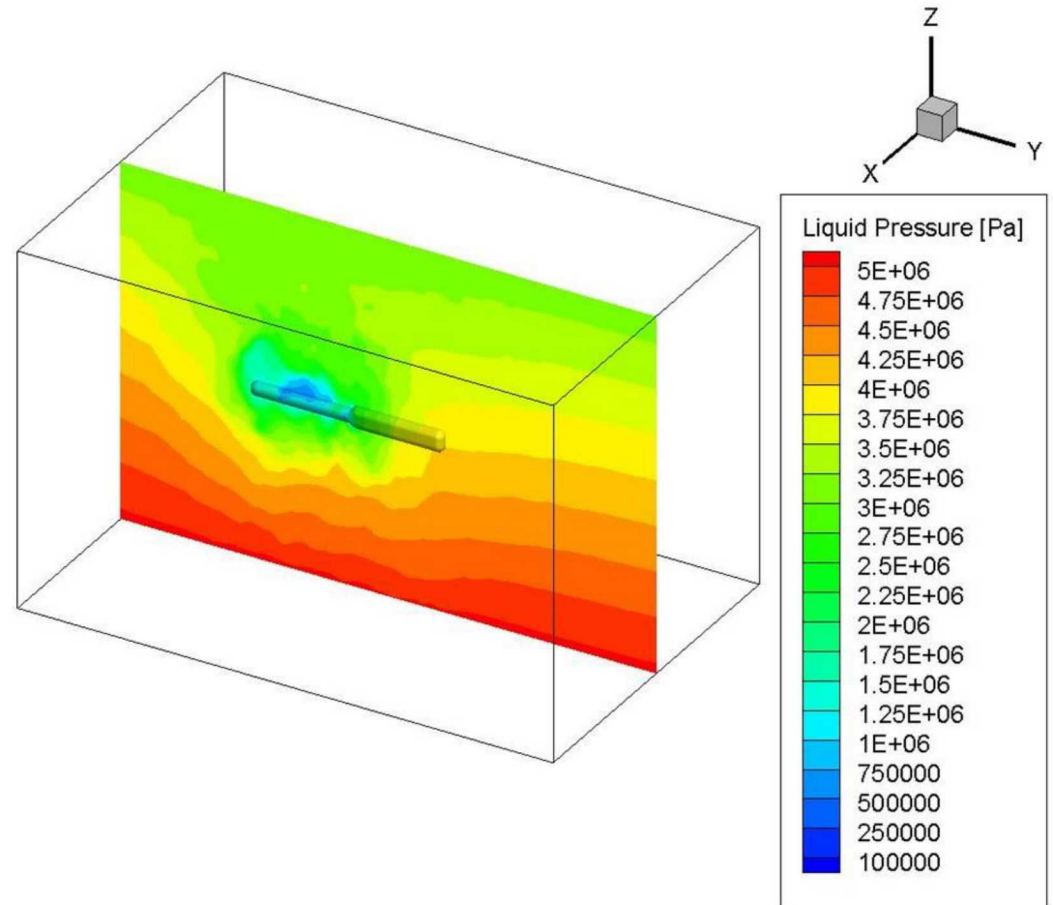
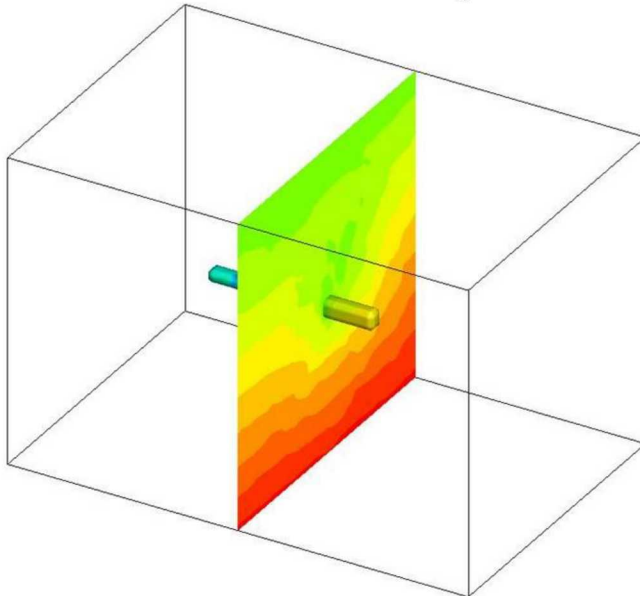
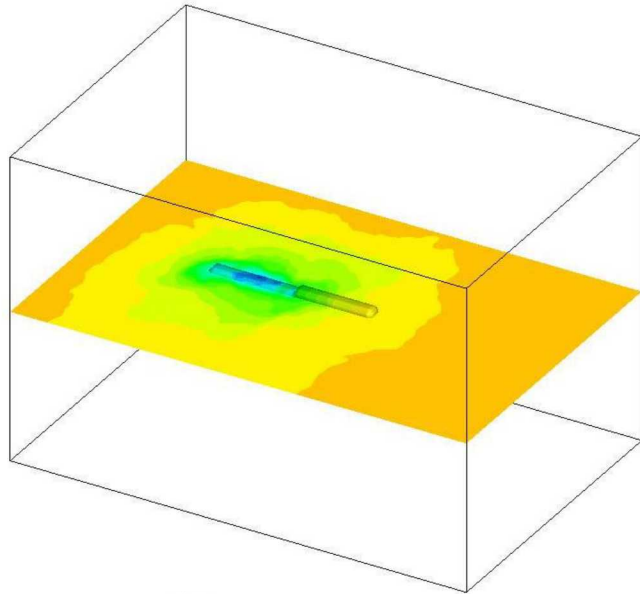


- Updated predictions of CTD filling and post-filling period.
- Run model to steady state with CTD and P1 to P6 pressure values set:
 - CTD = 1 atm.
 - P1 = 3.822 MPa P2 = 1.286 MPa
 - P3 = 1.76 MPa P4 = 3.48 MPa
 - P5 = 3.79 MPa P6 = 3.357 MPa
- Run flow model to one year (Start Jan. 7/2016) using steady state as initial condition.
 - Performed calibration analysis by adding injection and leakage at CTD-Inclined Tunnel side (where plug is).
 - Applied 0.0 flux boundary condition at other CTD walls.

Step2b: Steady State Pressure Distribution



Step2b: Pressure Distribution at End of Simulation Time (360 days)

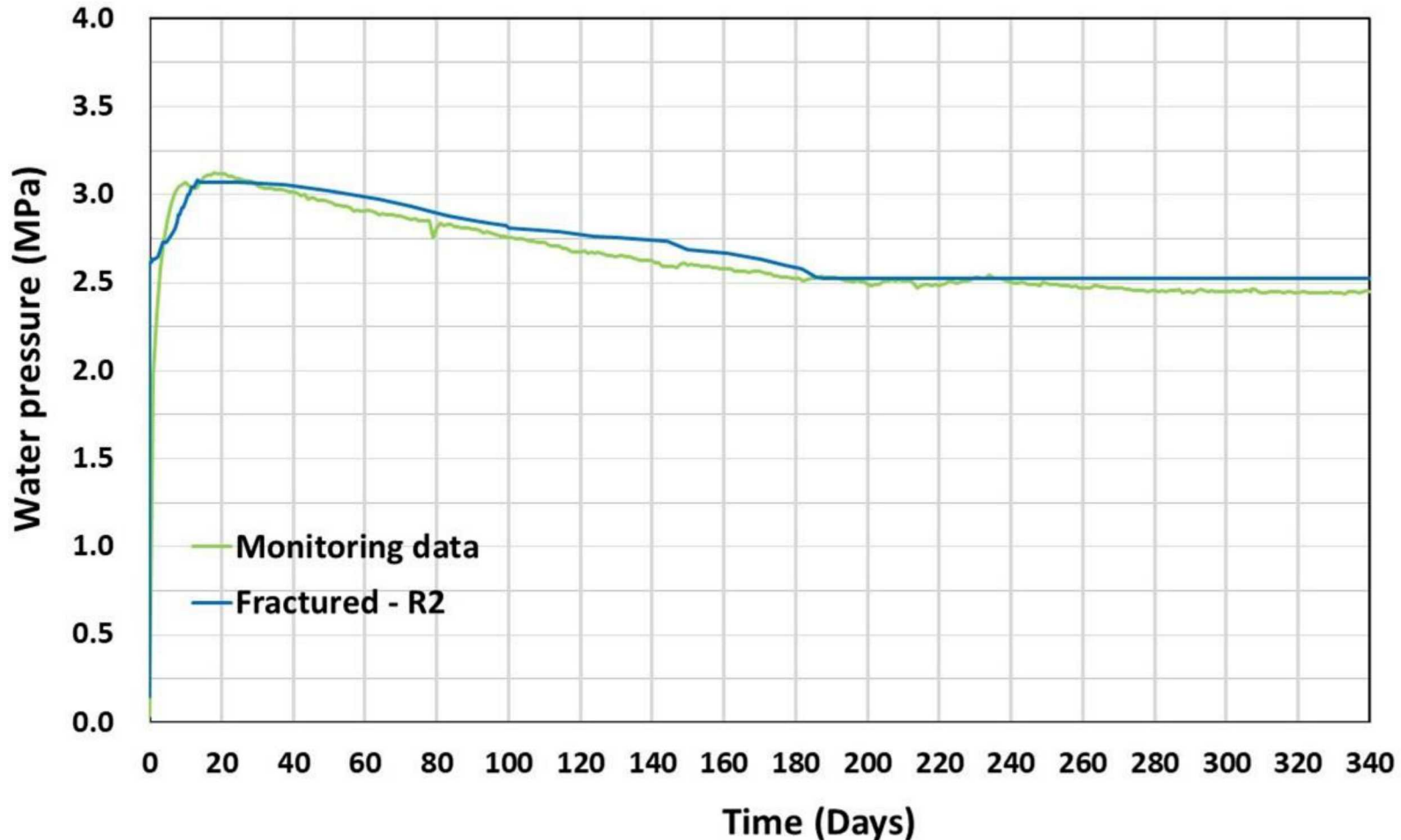


Fractured System: Realization 2

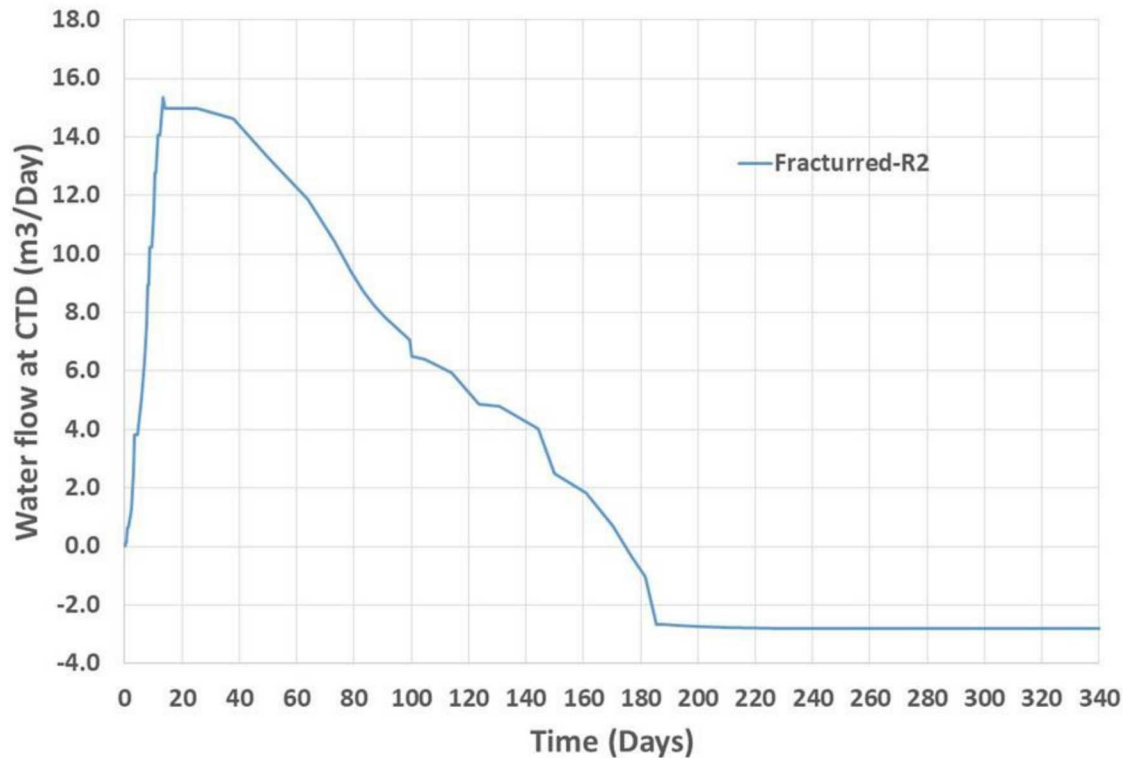
Step2b: Predicted Pressure History at CTD



Fractured System: Realization 2

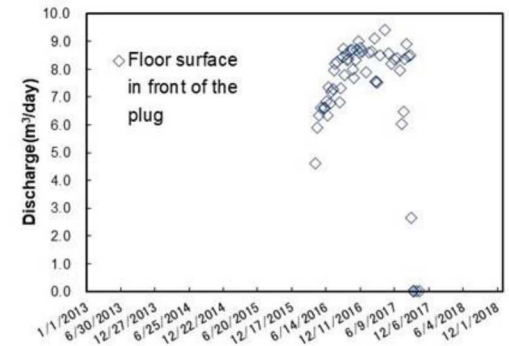


Step2b: Predicted Flow History at CTD: Filling and Leakage – Fractured System

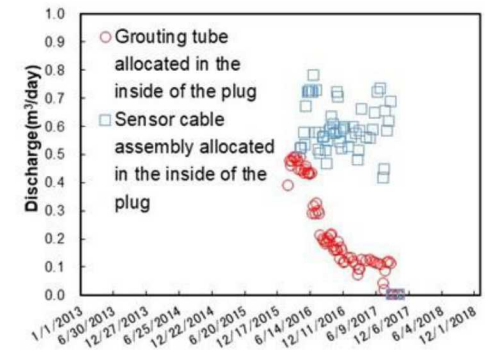


Predicted

Leakage from CTD



Leakage from CTD

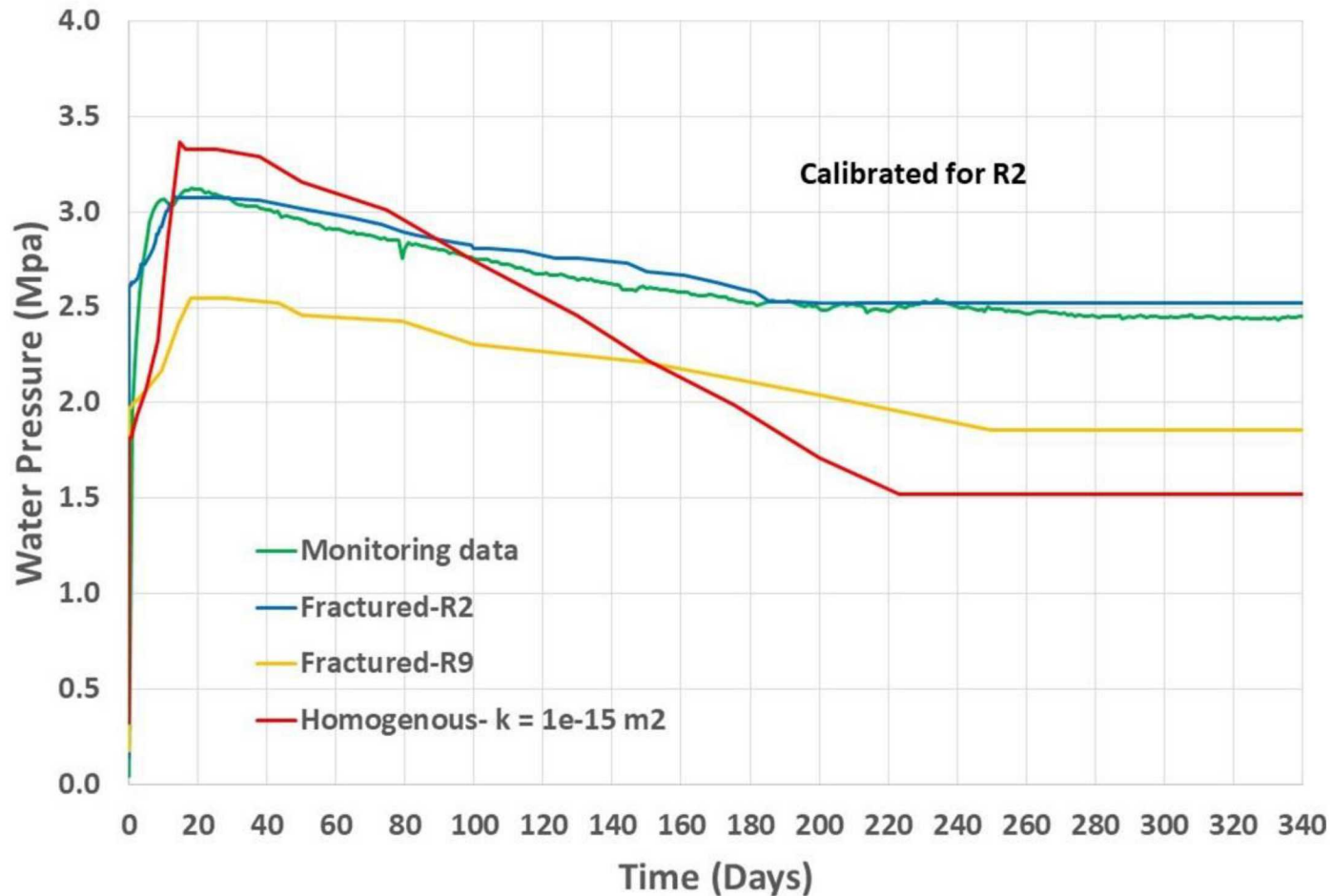


Experimental

Step2b: Predicted Pressure History at CTD: Fractured and Homogenous Systems



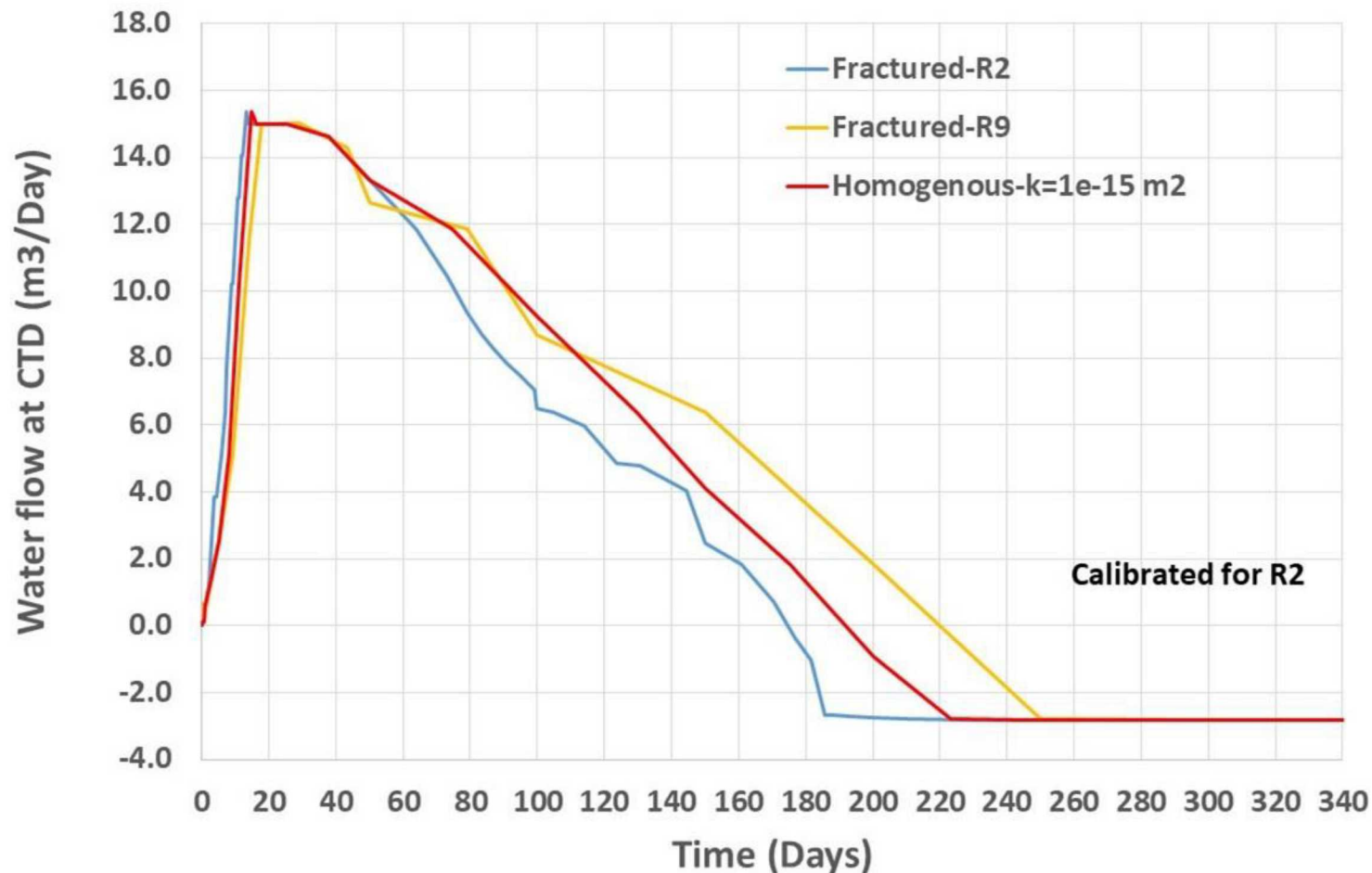
Fractured System: Realizations 2 and 9 and Homogenous System



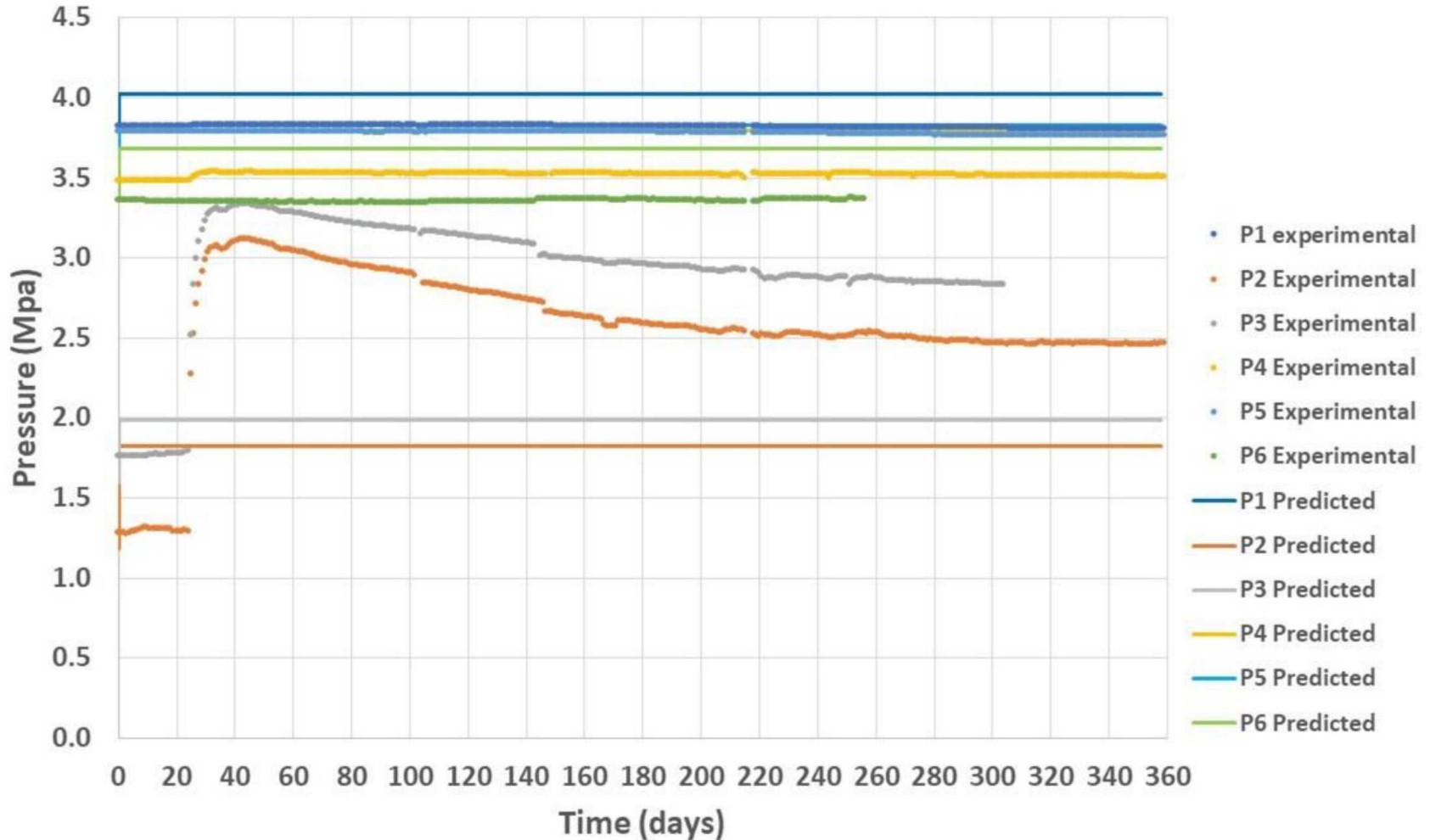
Step2b: Predicted Flow History at CTD: Filling and Leakage Amount



Fractured System: Realizations 2 and 9 and Homogenous System



Step2b: Predicted Pressure History at Observation Points in Well 12MI33

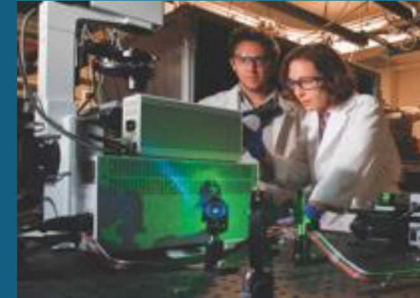


Part I Summary

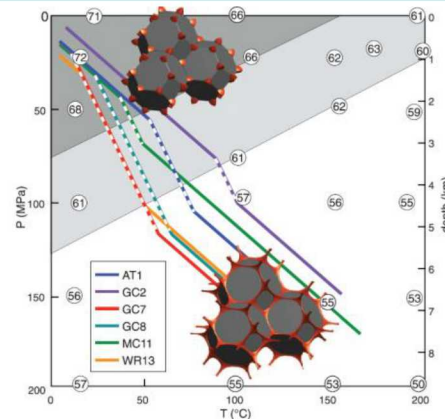
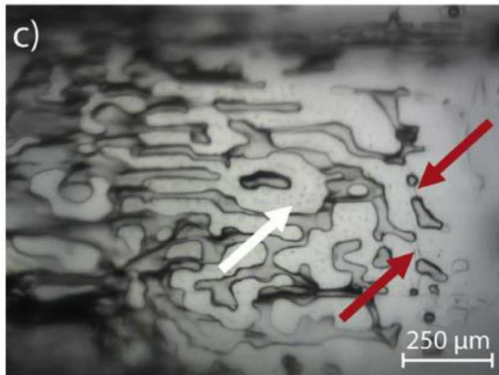


- Updated flow modeling was conducted for Task C, Step2b.
- The same domain and mesh as previous simulations were used.
 - The CTD-scale domain was enlarged to reduce boundary effects.
- Used Realization 2 fracture permeability and porosity fields as base case. Used Realization 9 and Homogenous system with permeability of 10^{-15} m^2 for sensitivity study.
- Conducted Modeled CTD filling and post-filling with the addition of injection and leakage from the CTD.
 - Conducted calibrations using experimental CTD pressure vs time data to determine injection and leakage amount.
 - Predicted pressure history in observation points in Well 12MI33. Predictions were reasonable for all except P2 and P3. Better matching of pressures in P2 and P3 is needed.

DECOVALEX19 TASK F: Fluid Inclusion and Movement in Tight Rocks (FINITO)



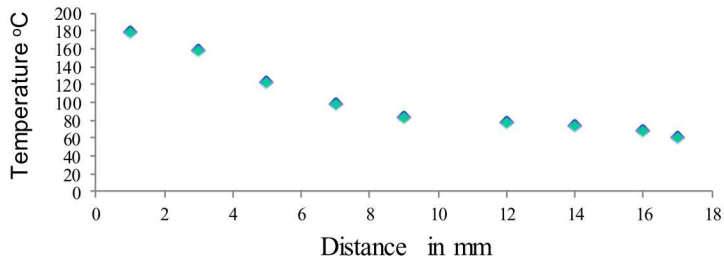
DECOVALEX19
WORKSHOP 6
Seoul, R. of Korea
Oct. 16-19, 2018



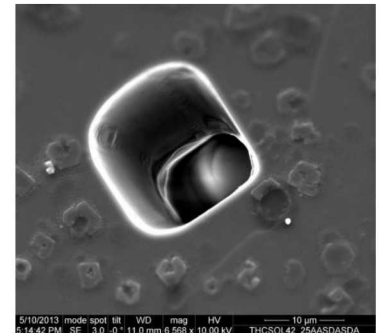
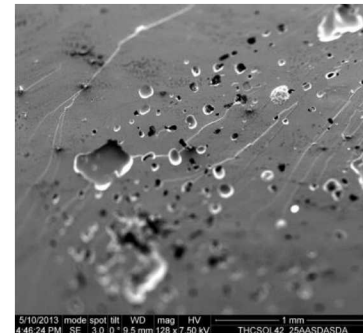
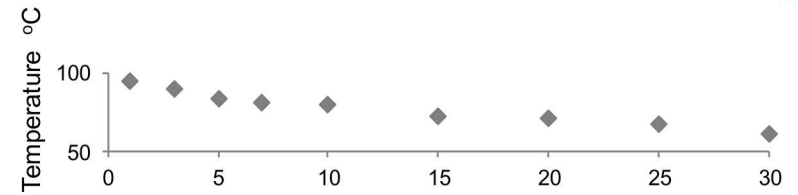
PRESENTED BY

Yifeng Wang (SNL)

Observations

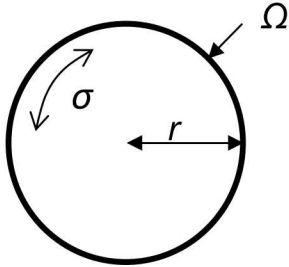


Caporuscio et al. (per. Comm.)



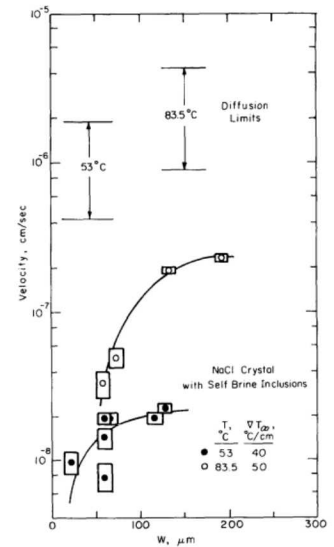
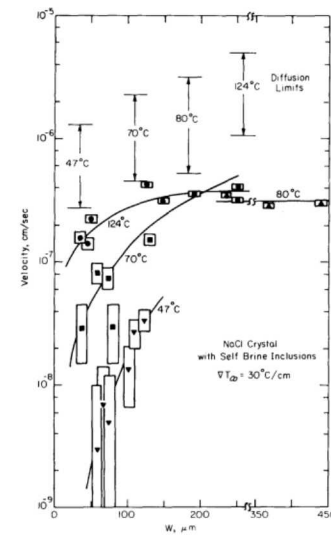
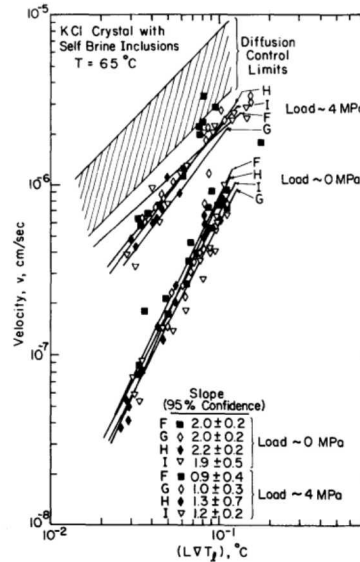
Interface instability and channeling

Migration of a single fluid inclusion



$$V_0 \approx \frac{V_m D K_d^0 \Delta H_r \alpha}{RT_0^2} e^{-\frac{2\gamma V_m}{RT_0 r}}$$

$$K_d^0 \propto e^{\frac{\Delta H_r}{RT_0} + \frac{\beta V_m \sigma^2}{RT_0}}$$



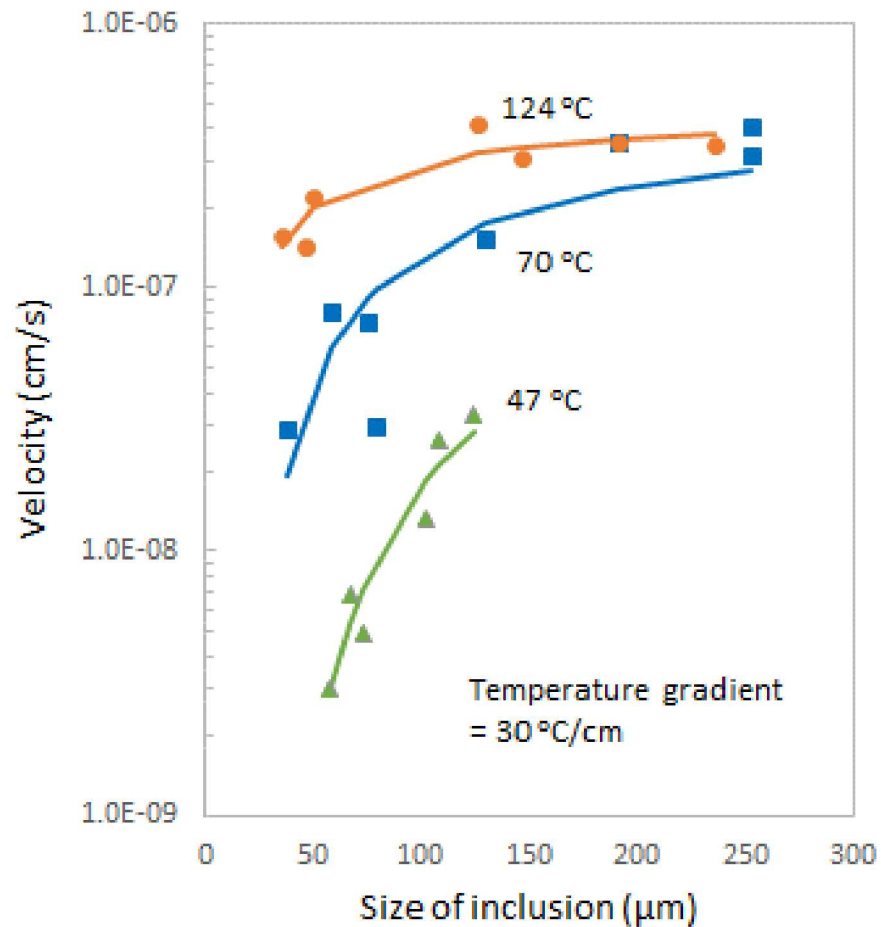
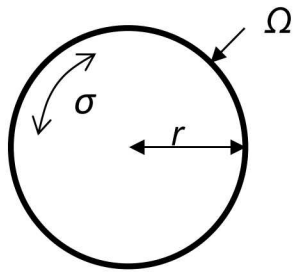
Wang (2017)

$$D \propto e^{\frac{\Delta E}{RT_0}}$$

Data from Olander et al. (1982)



$$V_0 \approx \frac{V_m D K_d^0 \Delta H_r \alpha}{R T_0^2} e^{-\frac{2\gamma V_m}{R T_0 r}}$$



Data from Olander et al. (1982)

Linear stability analysis



$$x > f(y, t):$$

$$\nabla^2 T_s = 0$$

$$x < f(y, t):$$

$$\nabla^2 T_l = 0$$

$$\nabla^2 m = 0$$

$$x = f(y, t):$$

$$R_d = k_d \left[K_d e^{-\frac{H}{R} \left(\frac{1}{T} - \frac{1}{T_0} \right) - \frac{2\gamma V_m \kappa}{RT_0}} - m \right]$$

$$-D \nabla m \cdot \vec{n} = R_d$$

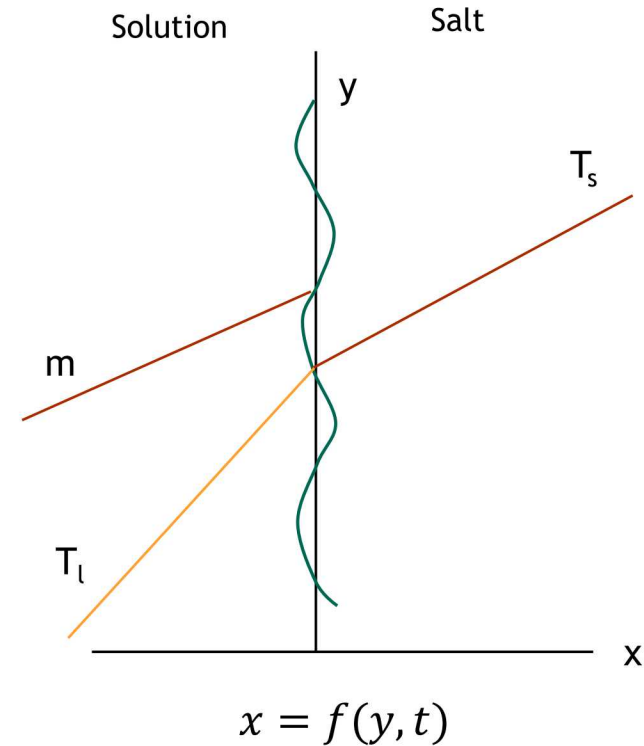
$$k_s \nabla T_s \cdot \vec{n} = k_l \nabla T_l \cdot \vec{n}$$

$$\vec{n} = - \left(\frac{\partial f}{\partial y} \right) / \left[1 + \frac{\partial f^2}{\partial y} \right]^{1/2}$$

$$\vec{n} = - \left(\frac{\partial f}{\partial y} \right) / \left[1 + \frac{\partial f^2}{\partial y} \right]^{1/2}$$

$$= - \frac{\partial^2 f}{\partial y^2} / \left[1 + \frac{\partial f^2}{\partial y} \right]^{1/2}$$

$$\frac{\partial f}{\partial t} = V_m R_d \left[1 + \frac{\partial f^2}{\partial y} \right]^{1/2}$$





$$T_s = \bar{T}_s + \delta T_s$$

$$T_l = \bar{T}_l + \delta T_l$$

$$m = \bar{m} + \delta m$$

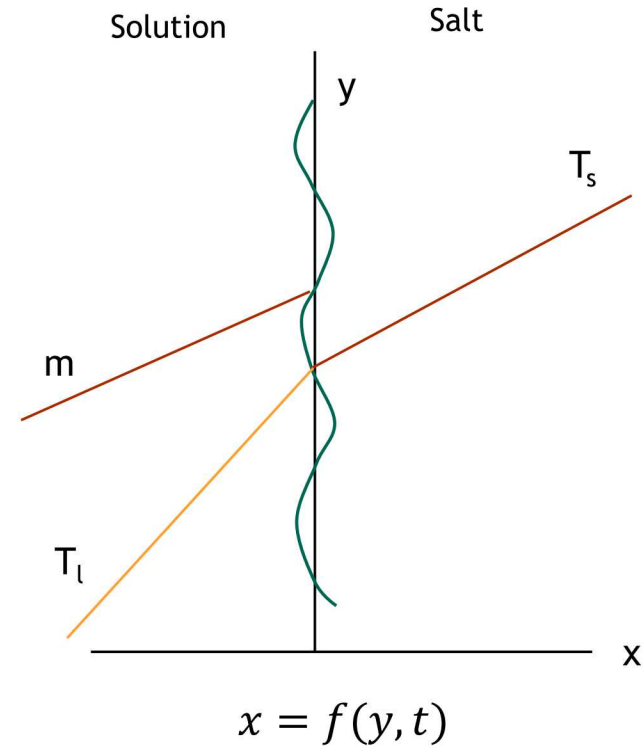
$$f = \delta f$$

$$\delta T_s = \hat{T}_s(s) e^{\xi t} \cos(\omega y)$$

$$\delta T_l = \hat{T}_l(s) e^{\xi t} \cos(\omega y)$$

$$\delta m = \hat{m}(s) e^{\xi t} \cos(\omega y)$$

$$\delta f = \hat{f} e^{\xi t} \cos(\omega y)$$



Result of linear stability analysis



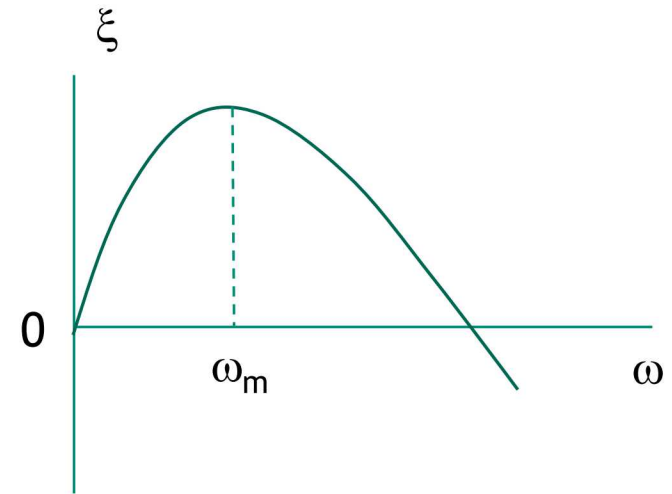
$$\xi = \frac{V_m D \omega \left(D \omega \frac{\partial \bar{m}}{\partial s} + \alpha k_d \frac{\partial \bar{T}}{\partial s} - \beta k_d \omega^2 \right)}{k_d + D \omega}$$

$$\frac{\partial \bar{T}}{\partial s} = \frac{k_s \frac{\partial \bar{T}_s}{\partial s} + k_l \frac{\partial \bar{T}_l}{\partial s}}{k_s + k_l}$$

$$\alpha = \frac{K_d H}{RT_0}$$

$$\beta = \frac{2\gamma V_m K_d}{RT_0}$$

Morphological instability causes the breakage of a large fluid inclusion.



For $k_d \rightarrow \infty$ (diffusion limited):

$$\xi = V_m D \omega \left(\alpha \frac{\partial \bar{T}}{\partial s} - \beta \omega^2 \right)$$

$$\omega_m = \sqrt{\frac{\alpha}{3\beta} \frac{\partial \bar{T}}{\partial s}}$$

$$\lambda = \frac{2\pi}{\omega_m}$$

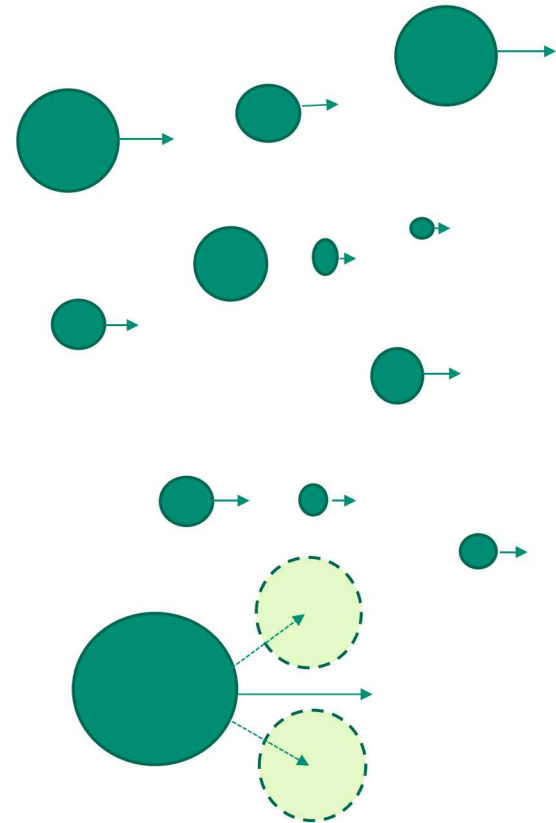
From individual inclusions to continuum scale fluid migration: A modeling scheme



$$\frac{\partial \rho(x, y, z, t; r)}{\partial t} = -\nabla \cdot [\vec{V} \rho(x, y, z, t; r)] + R_c - R_b$$

$$V_0 \approx \frac{V_m D K_d^0 \Delta H_r \alpha}{R T_0^2} e^{-\frac{2\gamma V_m}{R T_0 r}}$$

$$Q(x, y, z, t) = \int_0^\lambda \frac{4\pi}{3} r^3 \rho(x, y, z, t; r) dr$$



Possible chaotic behaviors of fluid release from rock salt

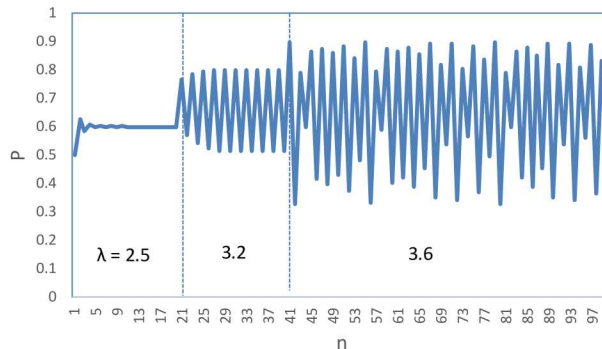
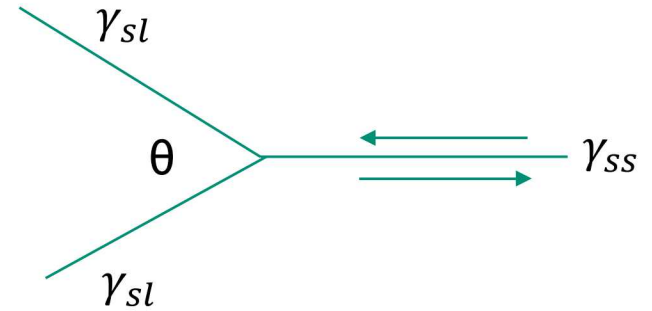


$$\cos\left(\frac{\theta}{2}\right) = \frac{\gamma_{ss}}{2\gamma_{sl}}$$

$$\frac{dS}{dt} = k_1 S - k_2 P S$$

$$p \propto S$$

$$\frac{dS}{dt} = k_1 S - k_2 S^2 = k_1 S(1 - k_2 S)$$



Possible chaotic behaviors of fluid release from rock salt

