Advancing CO2 and Hydrogen Storage in Lithuania: A machine learning and Digital Rock Physics Approach

Mayur Pal| GeoEnergy Lab @ MLAB – KTU, Lithuania

2025-03-25 – ECO AI workshop, Heriot-Watt University

Kaunas University of Technology, Lithuania

GeoEnergy Lab @MLAB

KTU - AI Centre

GeoEnergy Lab

Head of the Laboratory – Mayur Pal

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Priority research areas:

- Mathematical Modelling/Applied Mathematics
- Application of AI and ML Technologies
- Sustainable energy developments:
    - Geothermal
    - Hydrogen
    - CCS

Team Members:

- Pijus Makauskas, PhD Student (Subsurface modelling)
- Abdul Rashid, PhD Student (Geothermal)
- Shankar Lal, PhD Student (Hydrogen)
- Shruti Malik, Postdoctoral Researcher (CCS)
- Ieva Kaminskaite, Postdoctoral Researcher (Geothermal)
- Apoorv Verma, Postdoctoral Researcher (Hydrogen)
- Vaibhav Valmik, Masters student (AI and ML)
- Parsa Alimohammadiardakani, Bachelors (CCS, AI and ML)

Collaboration with National & International companies

GeoEnergy Lab

Research Thematic: **Carbon Capture Storage (CCS)**

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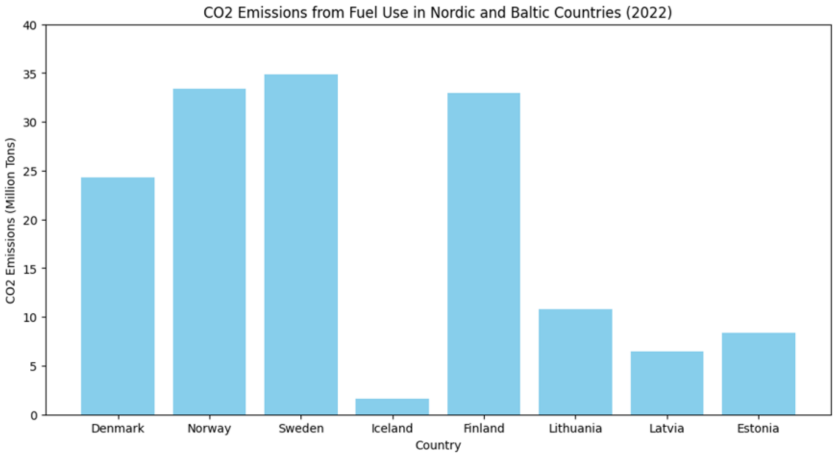
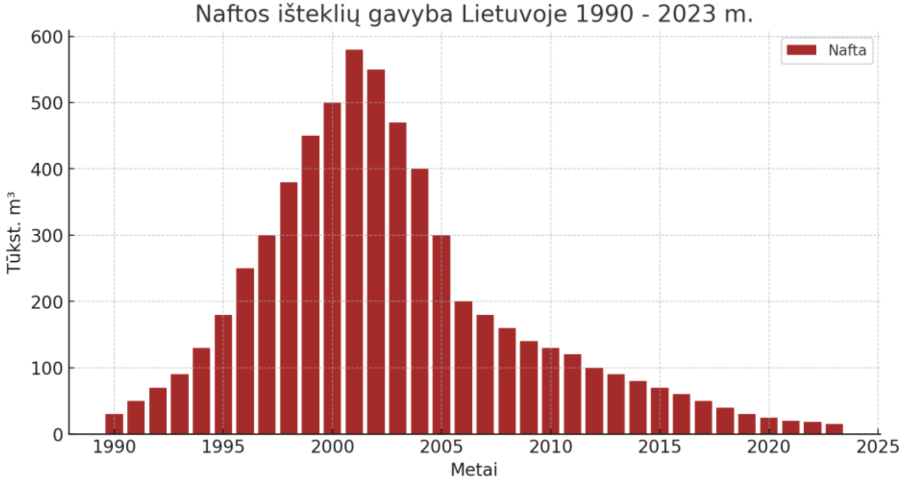
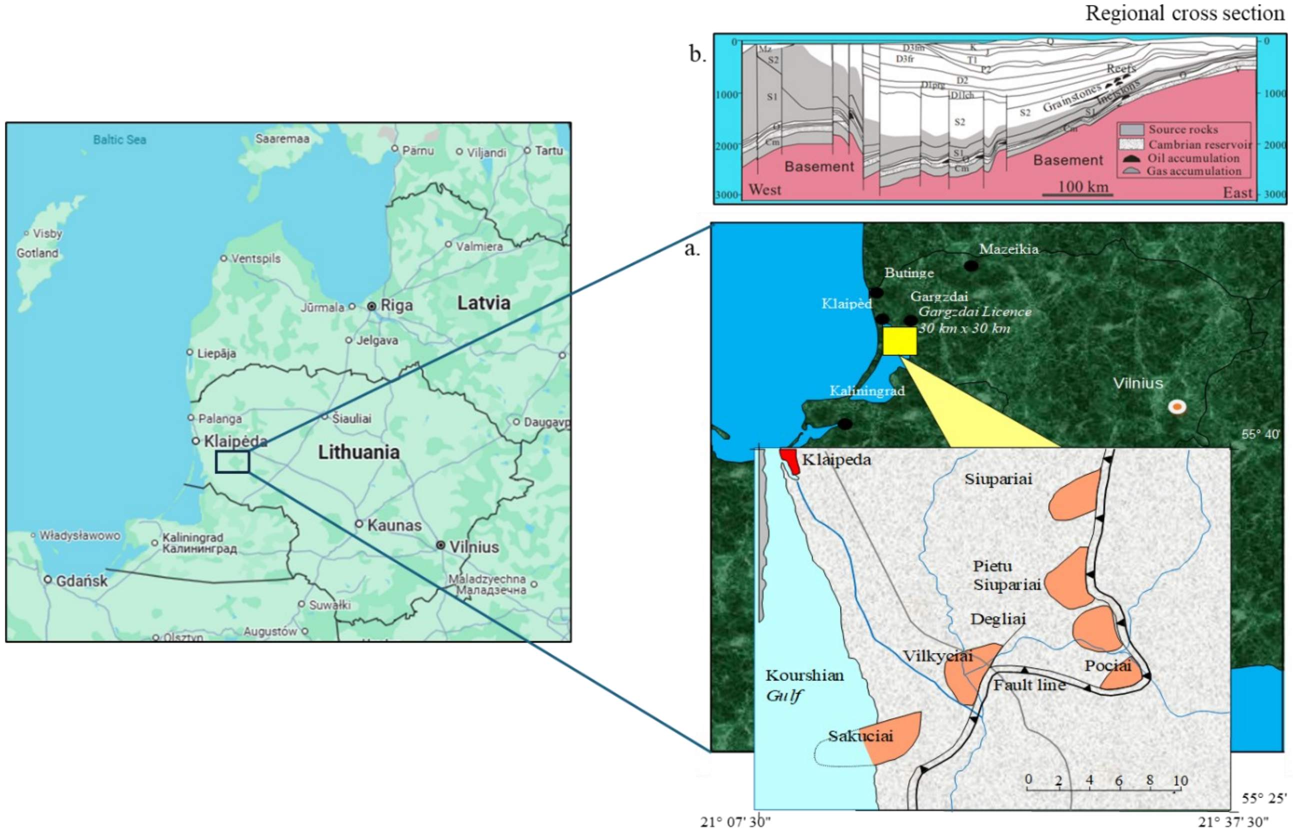
Context: Research area CCS

- Modelling and Experimental Analysis of Carbon Capture and Storage (CCS)







Successful CO2 Injection Pilot Test conducted

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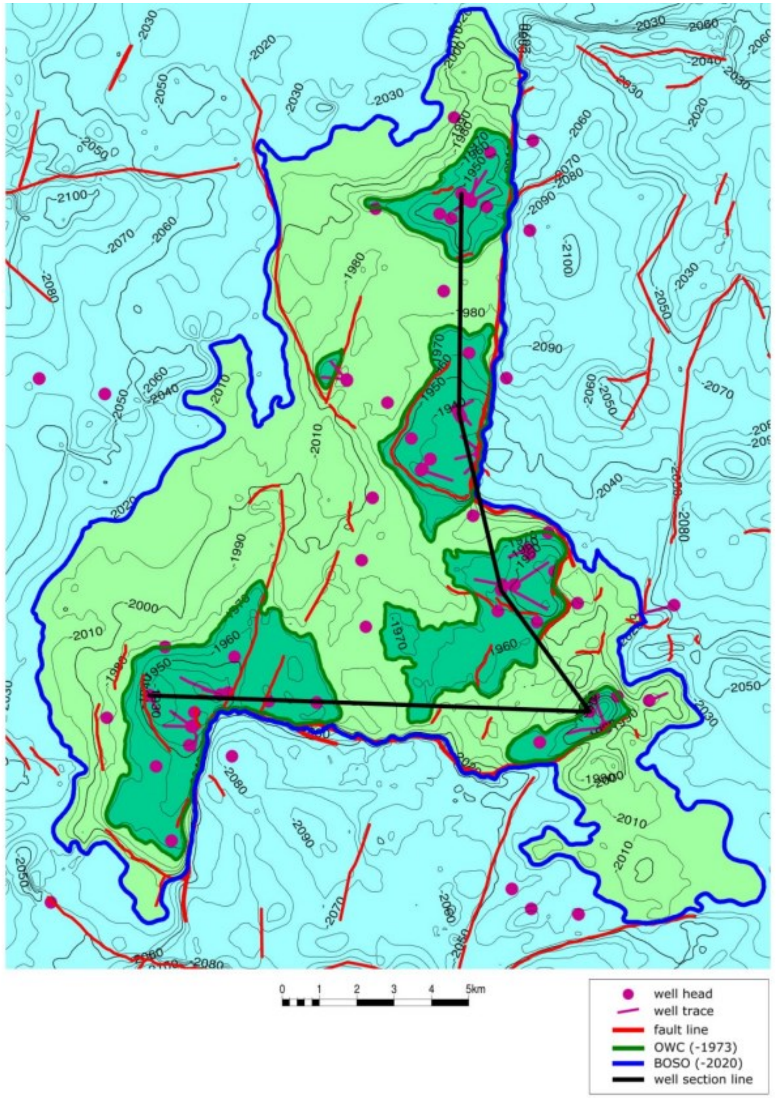
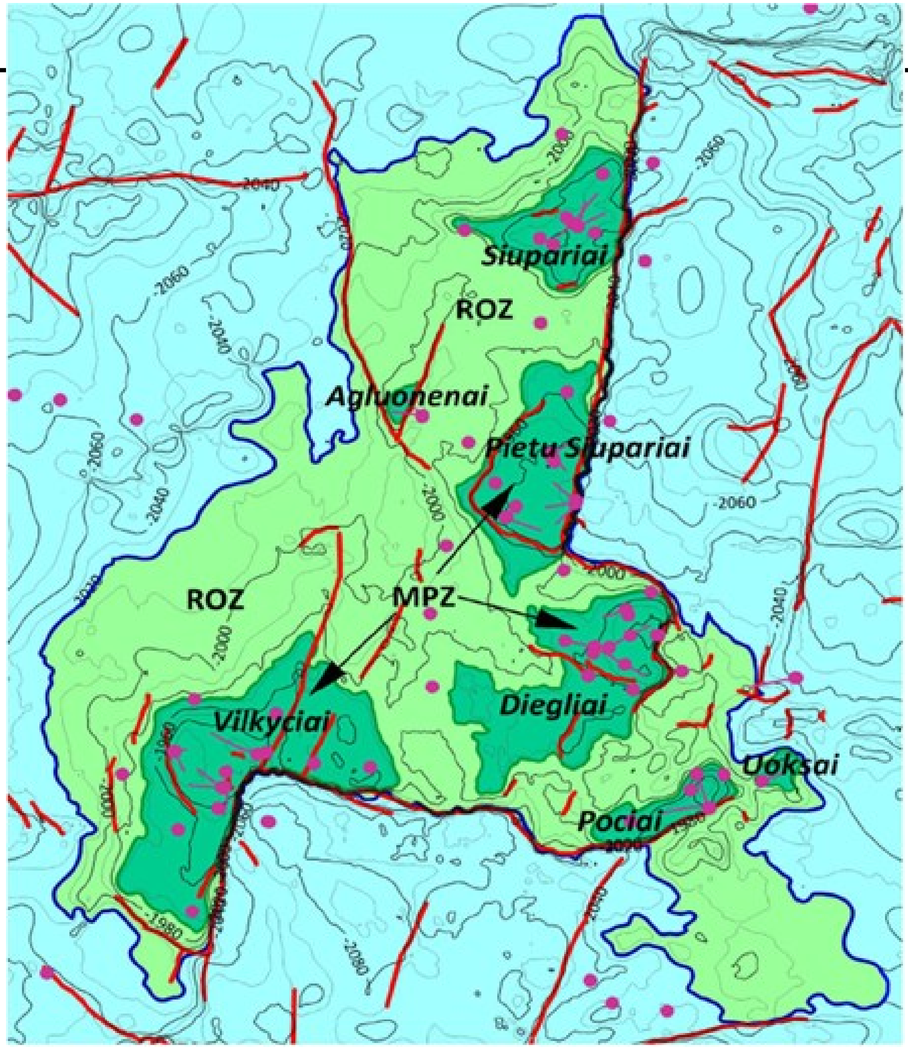
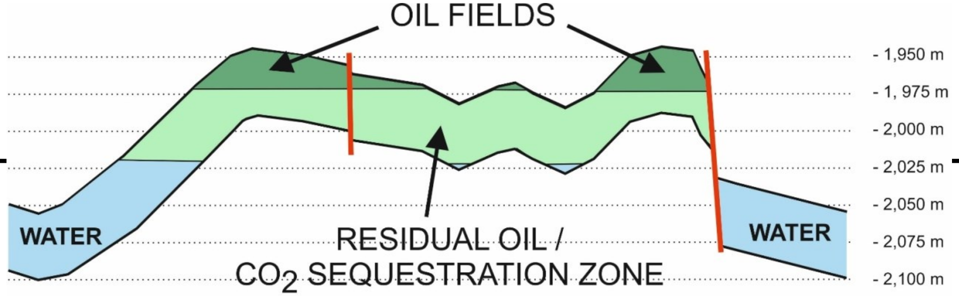


Working tank and pump with heater unit

Well	Injection Start	Injection Duration (days)	Injected CO_2 (tons)
DEG- 1	2013	49	988
PS-5	2014	2	40
POC-3	2015	2	40
PS-2A	2016	11	253

Carbon Capture Storage (CCS) in Gargzdai Residual Oil Zone





- Total area around 200- 245 Sq. Km, 100 m thick
- Gargzdai has large residual oil zone.
- Storage estimates around ~100 Mln Tons*
- **Proper modelling and experimental assessment is required for storage capacity and risk assessment for long term storage**

Malik, Shruti; Makauskas, Pijus; Karaliūtė, Viltė; Pal, Mayur; Sharma, Ravi. Assessing the geological storage potential of CO2 in Baltic Basin: a case study of Lithuanian hydrocarbon and deep saline reservoirs // International journal of greenhouse gas control. London : Elsevier. ISSN 1750-5836. eISSN 1878-0148. 2024, vol. 133, art. no. 104097, p. 1-16. DOI: 10.1016/j.ijggc.2024.104097.

What does it involve ?

Subsurface flow modelling and Experimental Investigations

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Modelling & simulation of subsurface flow

$$\nabla \cdot (K \times \nabla \phi) = S\dot{\phi} - Q$$

Recharge rate: Q

Potential time derivative: $\dot{\phi}$

Storage coefficient: $S = \frac{-\Delta V_w}{\Delta x \Delta y \Delta h}$

$$\frac{\partial(\phi \rho_\alpha s_\alpha)}{\partial t} + \nabla \cdot \{\rho_\alpha u_\alpha\} = \frac{q_\alpha}{\rho_\alpha}$$

Each phase α *has its:*

Source: q_α

Density: ρ_α

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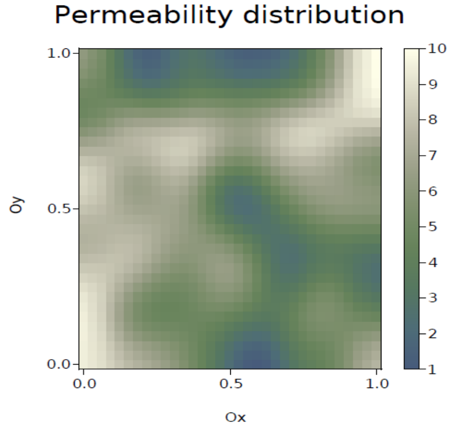
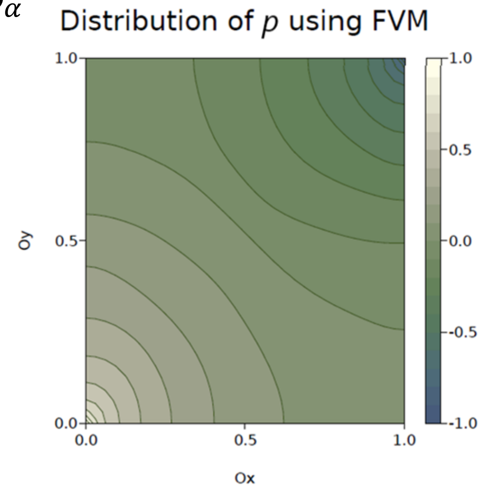
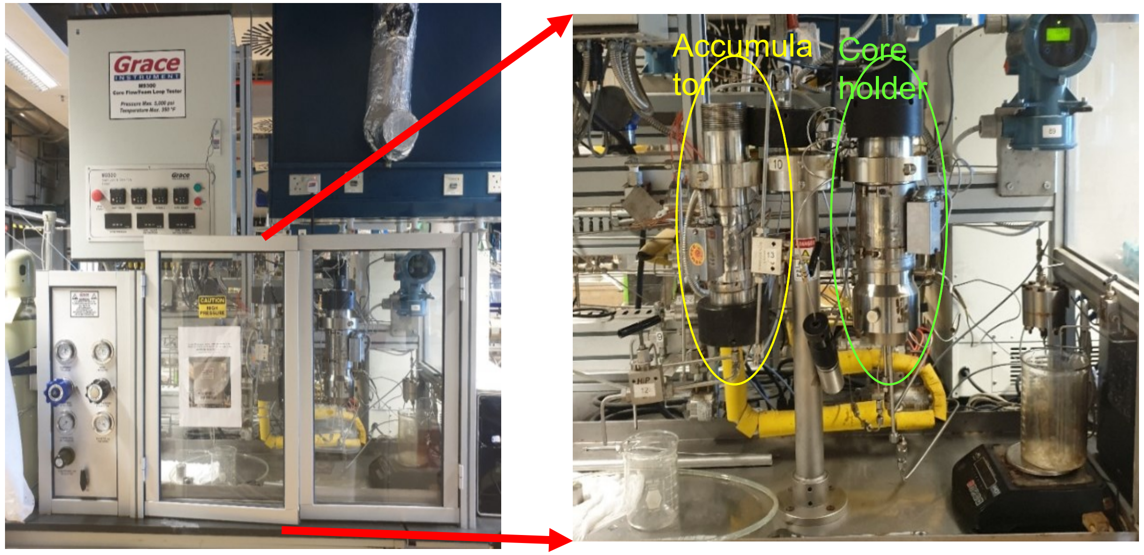


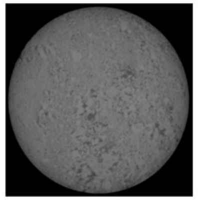


(b)

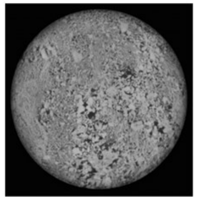
Experimental Investigations



The Core FlowLoop Tester instrument (left) and the accumulator and core holder within the closed chamber of the instrument (right) (Grace Instruments).



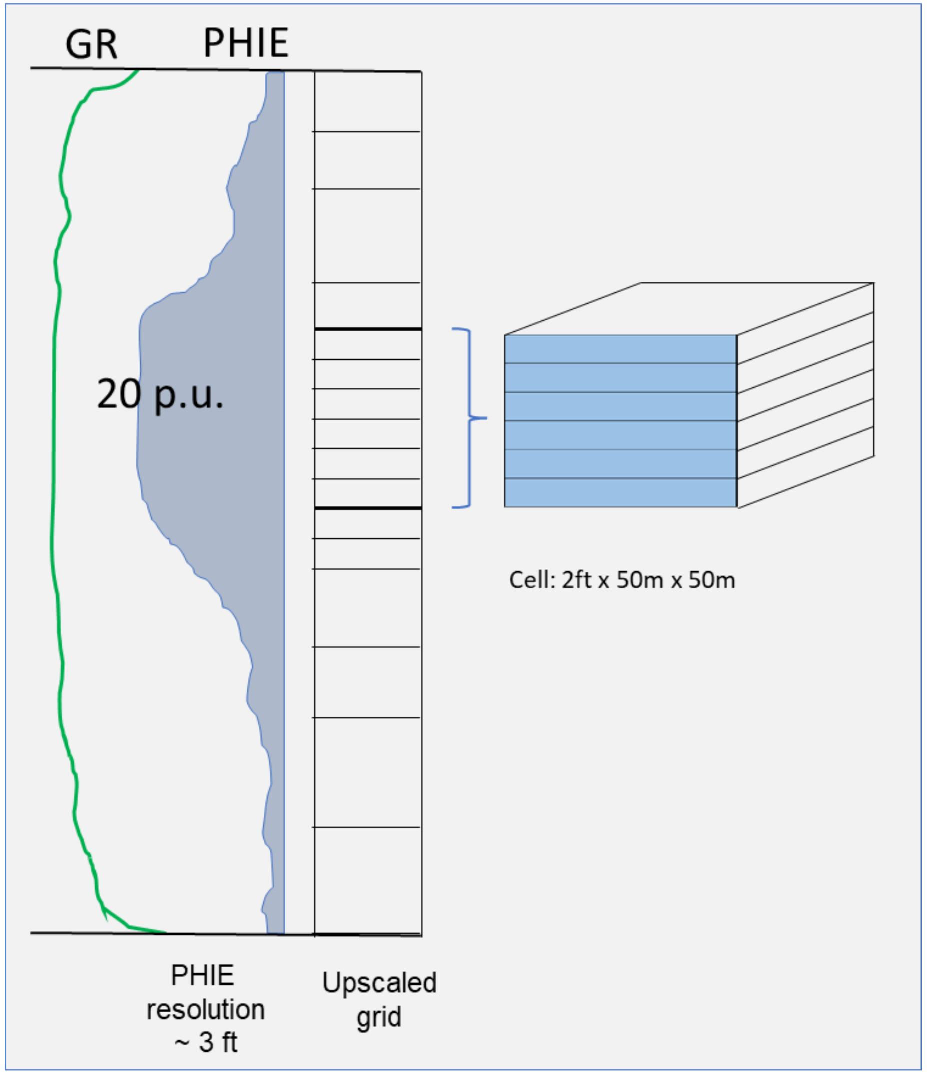
Original Image

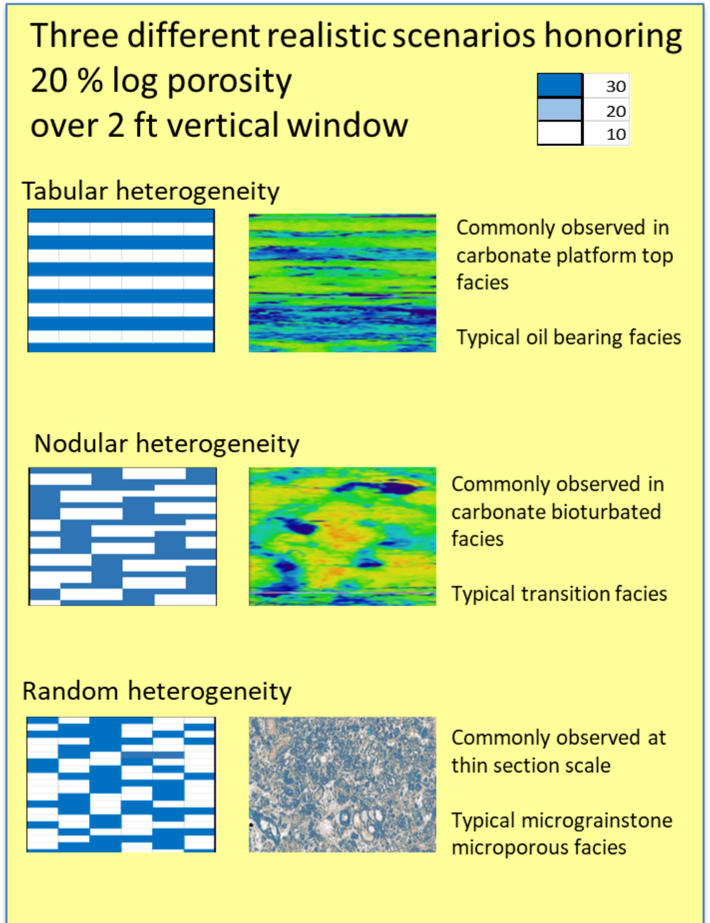


Contrast Limited Adaptive Histogram Equalization (CLAHE) adjusted Image

Why is it important ?

Impact of Heterogeneity on Subsurface Flow





All these textures can be described in a geostatistical sense, and implemented and tested in a box model.

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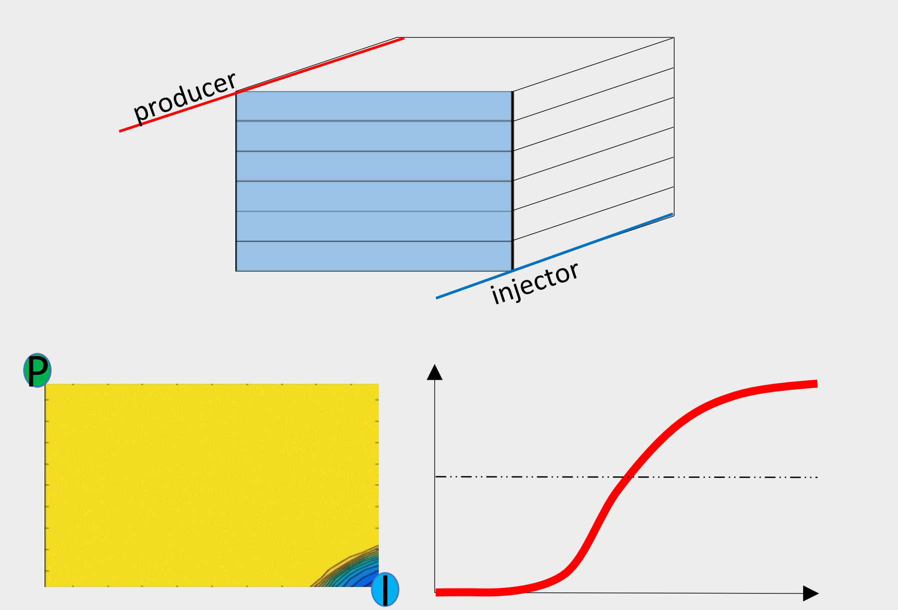
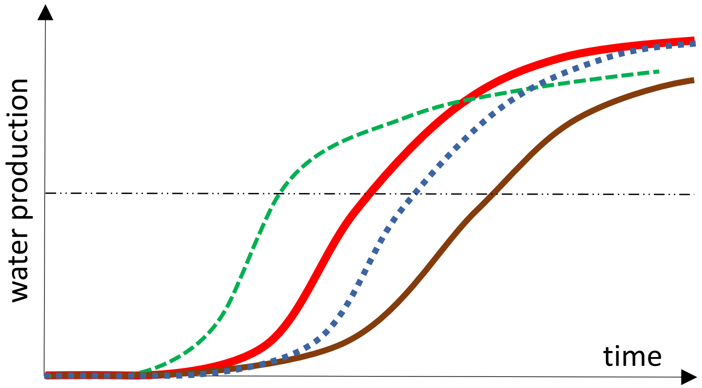
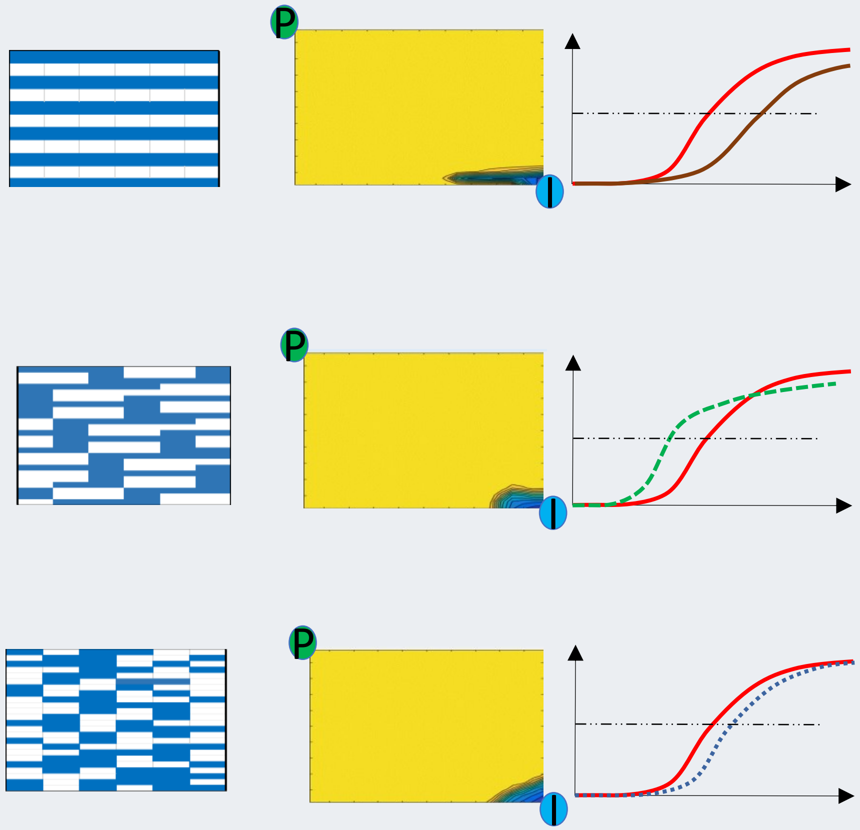
Impact of Heterogeneity on Subsurface Flow



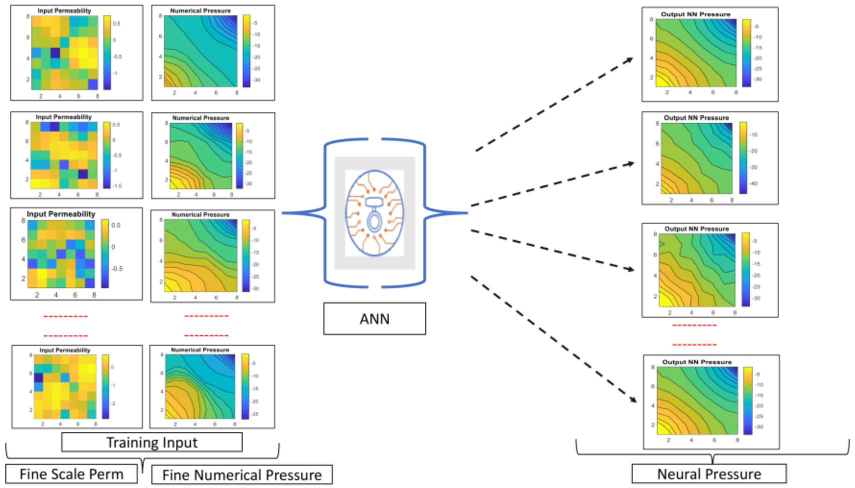
The log-derived uniform scenario

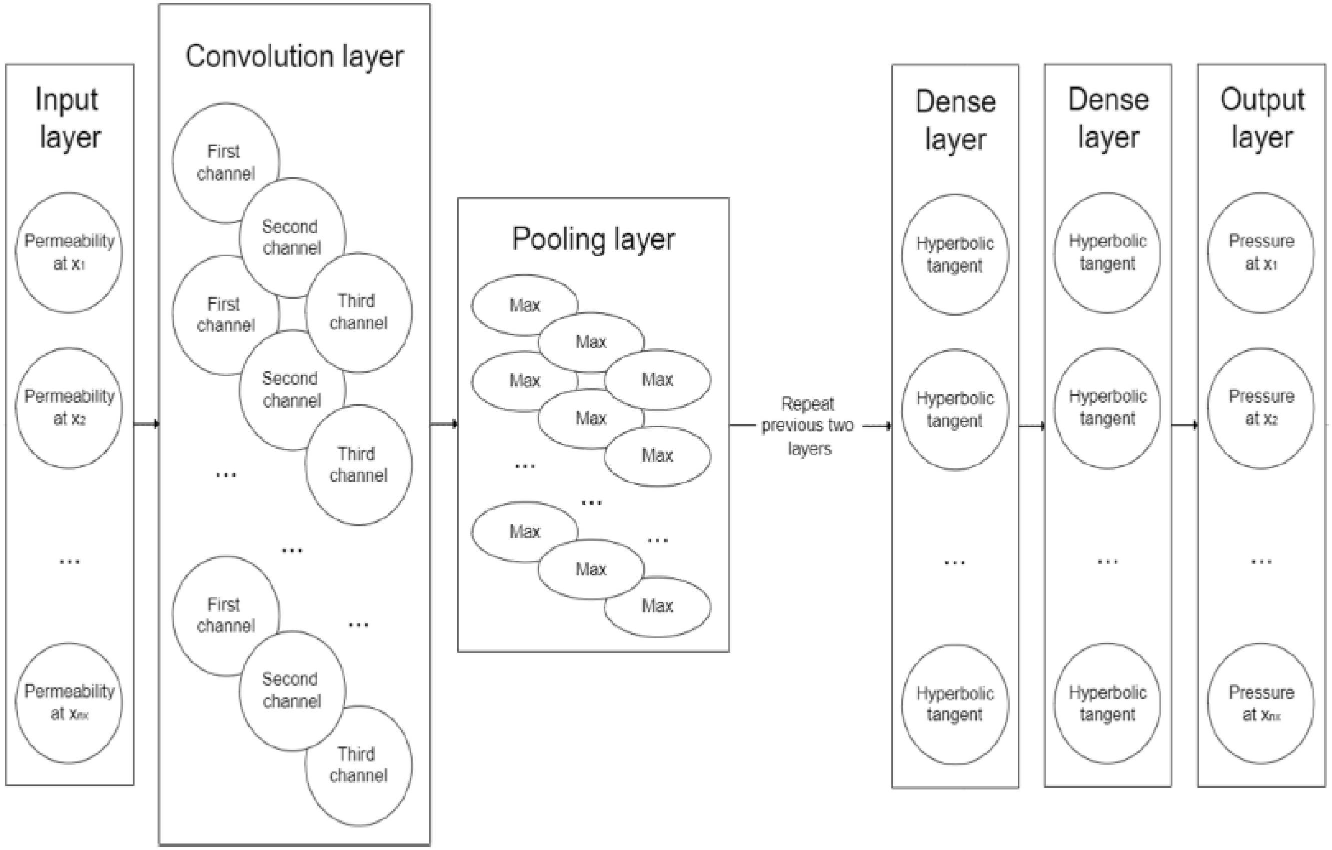




Various possible scenarios that can be deterministically defined by proper reservoir characterization

Neural Solutions of Elliptic Pressure Equation*





*Pijus Makauskas and Mayur Pal, Comparative study of modelling flows in porous media for engineering applications using finite volume and artificial neural network methods, Journal of Engineering with Computers, 2023, DOI:10.1007/s00366-023-01814-x

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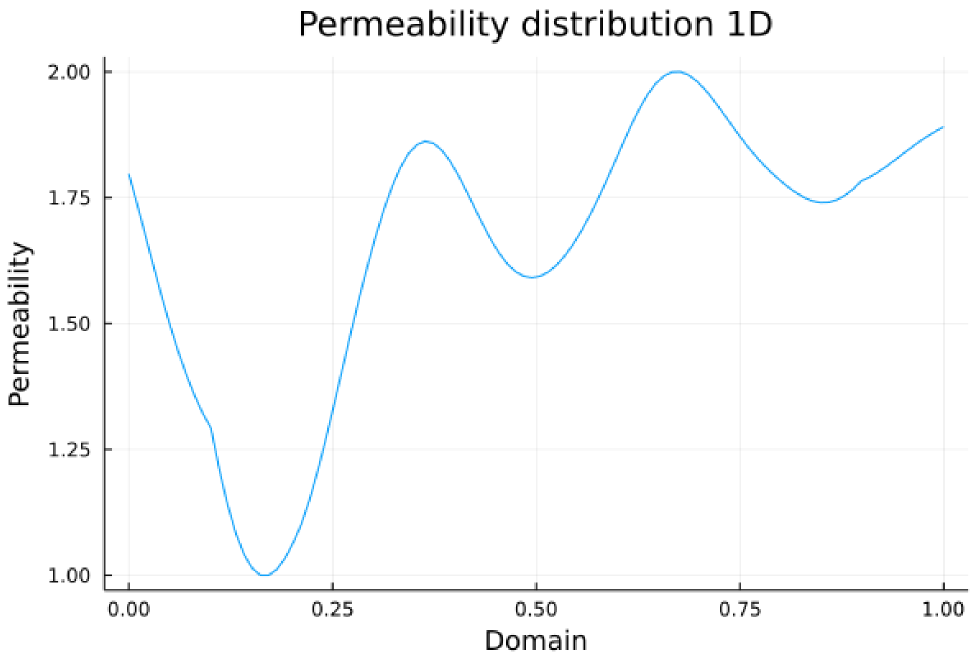

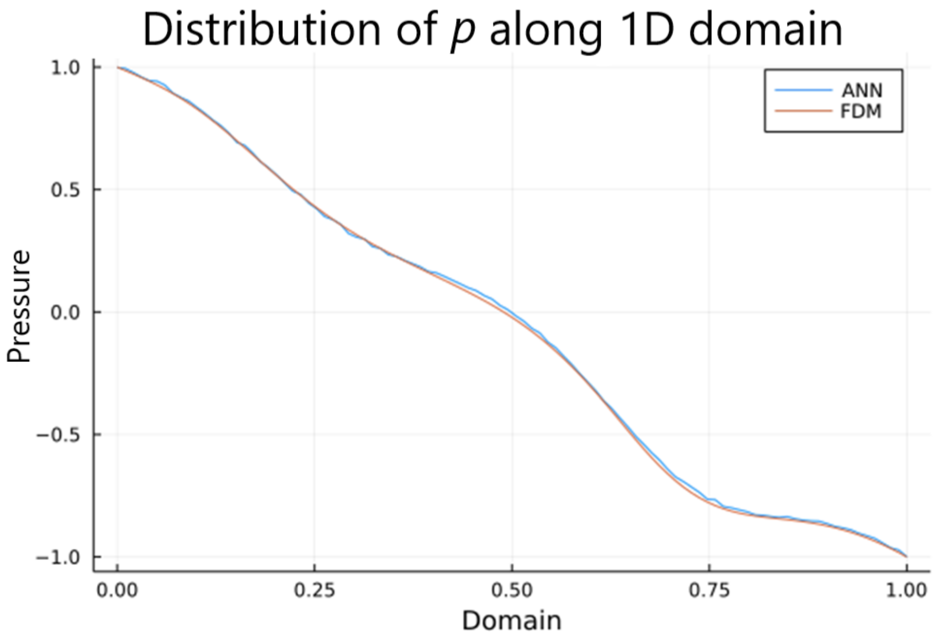

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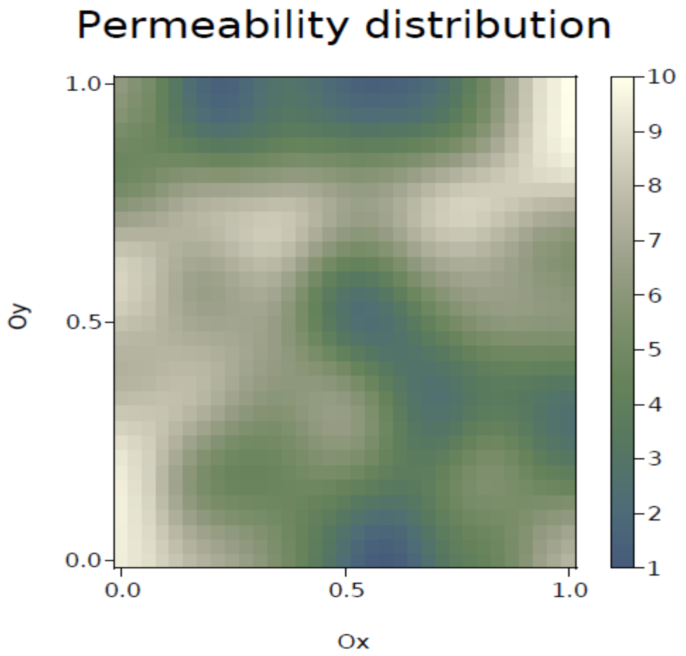

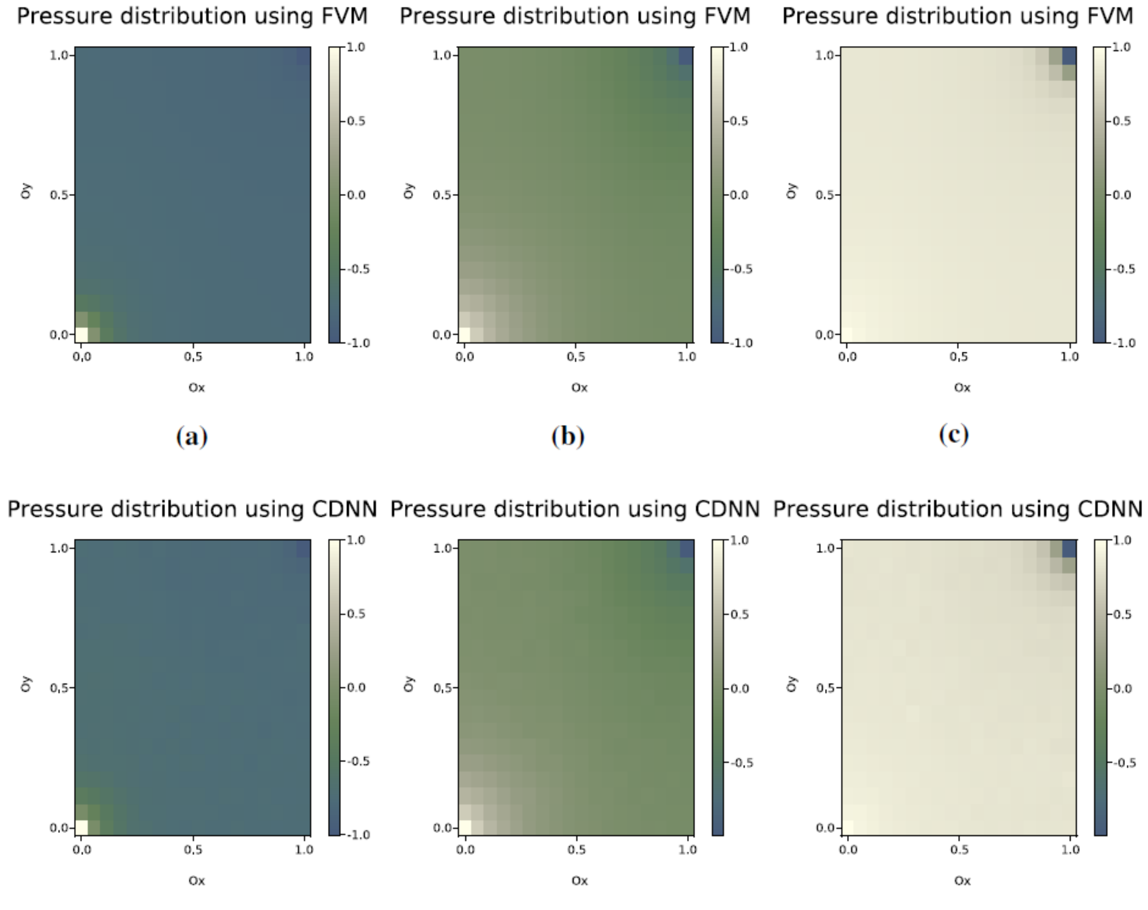

(a) (b) (c)

(d) (e) (f)

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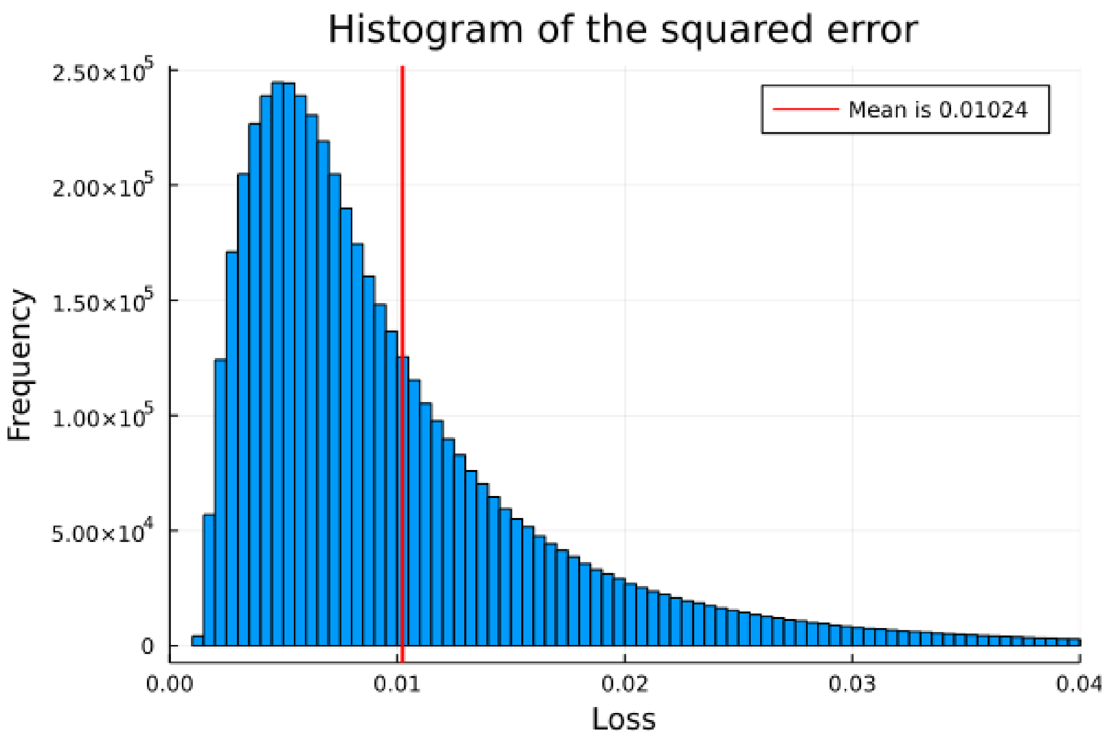

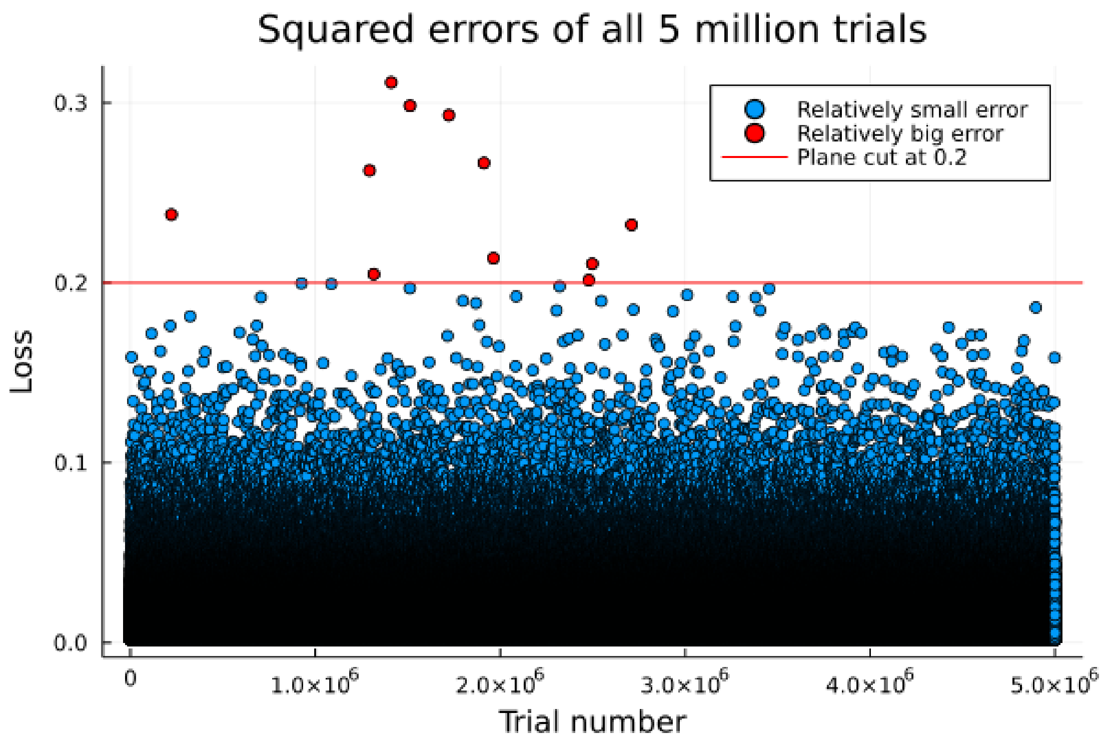

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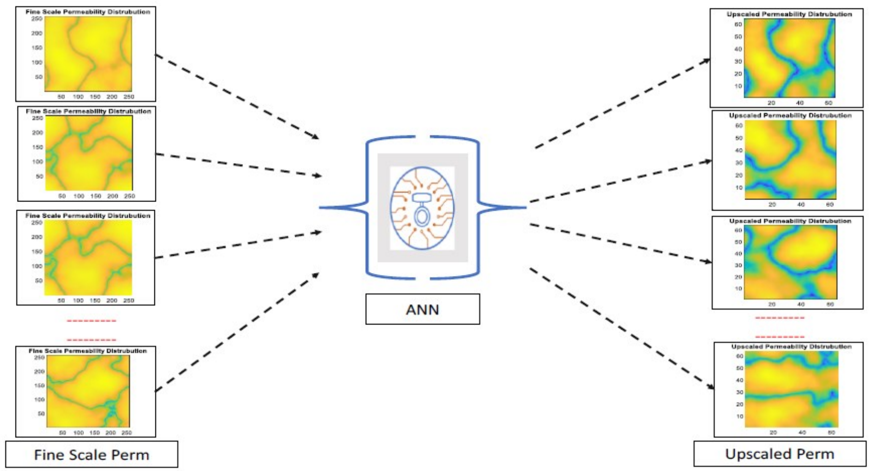
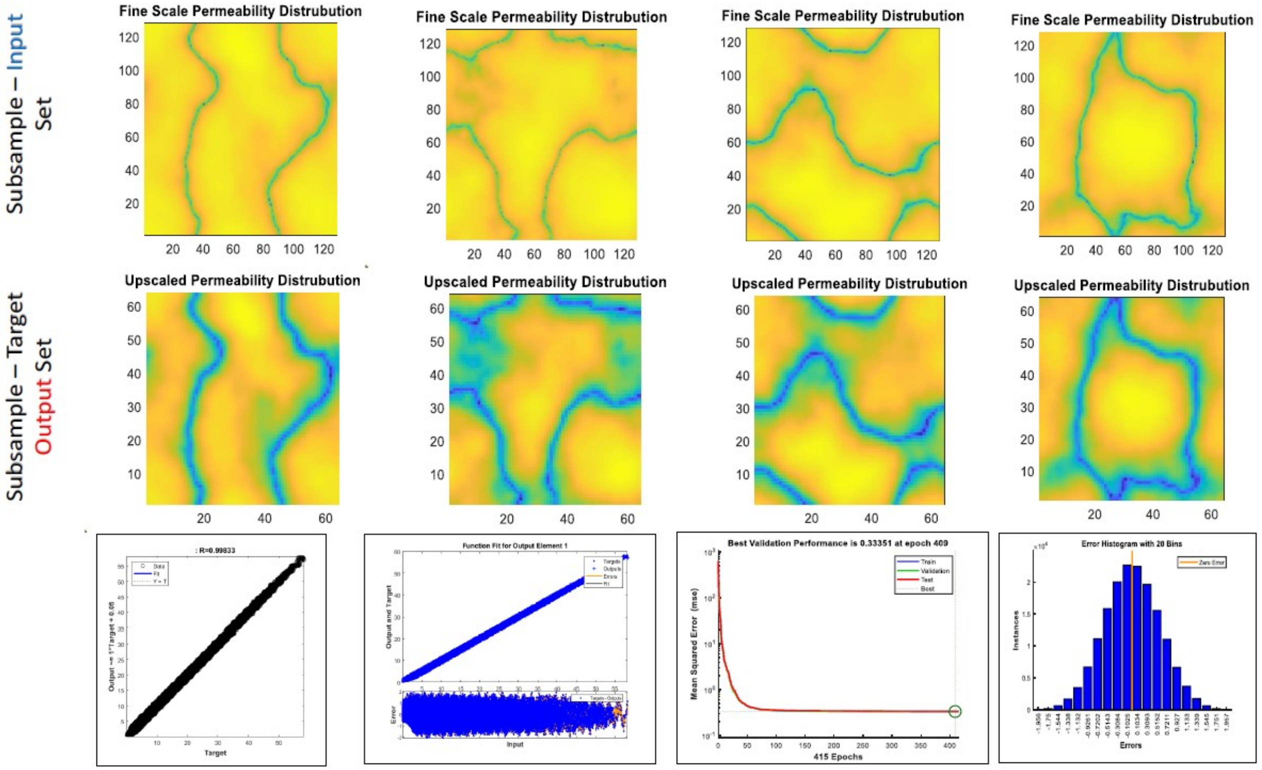
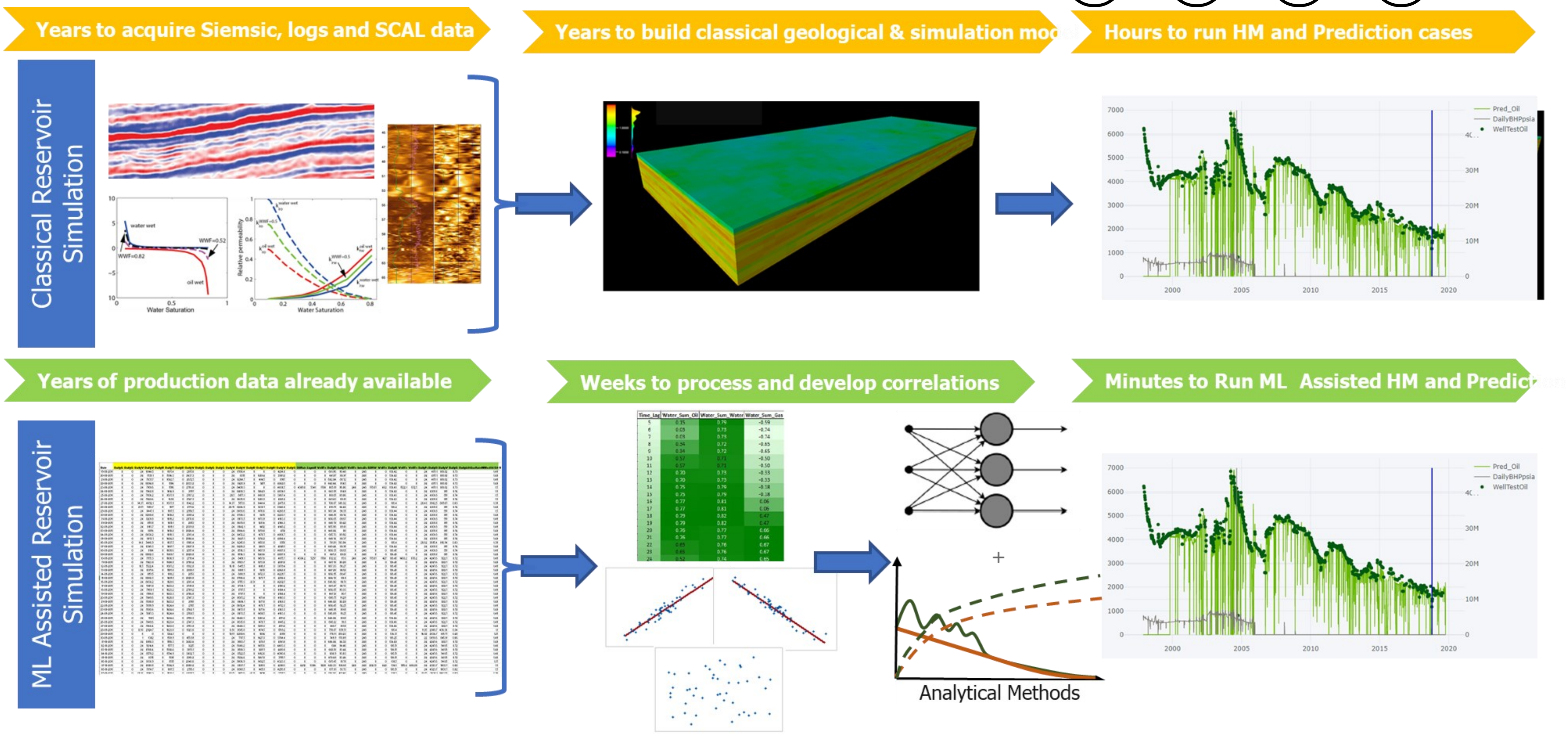
Neural Upscaling of Permeability Field*





*Pal, Mayur; Makauskas, Pijus; Malik, Shruti. Upscaling porous media using neural networks: a deep learning approach to homogenization and averaging // Processes. ISSN 2227-9717. 2023, vol. 11, iss. 2, art. no. 601, p. 1-21. DOI: 10.3390/pr11020601.

Research Topic Highlights – AI and ML in subsurface Modelling*



Pal, Mayur. On application of machine learning method for history matching and forecasting of times series data from hydrocarbon recovery process using water flooding // Petroleum science and technology. ISSN 1091-6466. eISSN 1532-2459. 2021, vol. 39, iss. 15-16, p. 519-549. DOI: 10.1080/10916466.2021.1918712.

Dicelytics Platform – AI & ML for Oil and Gas

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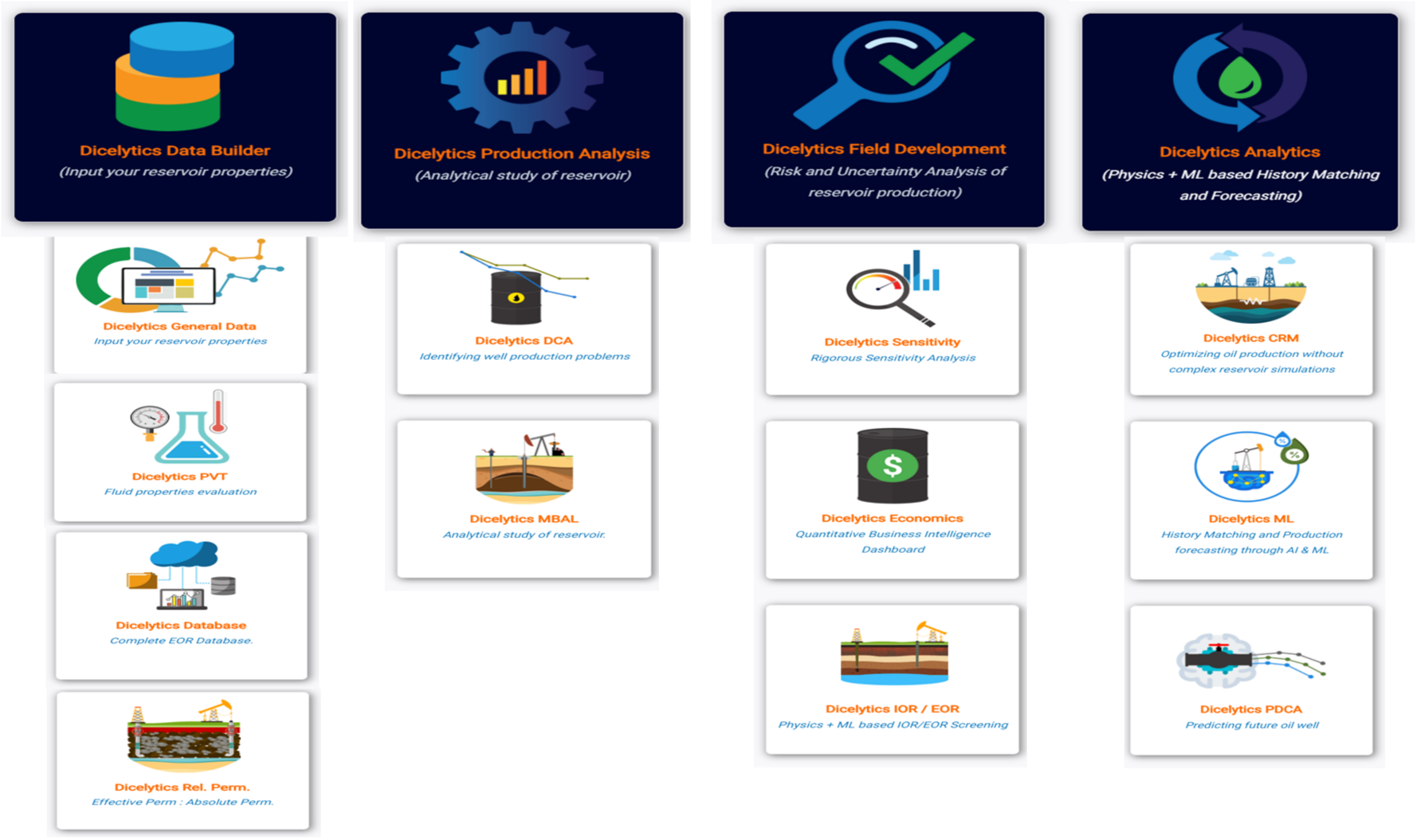

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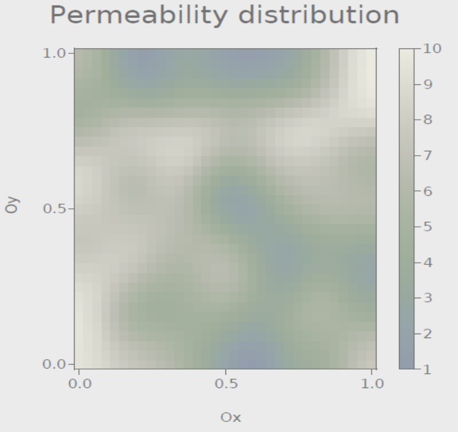
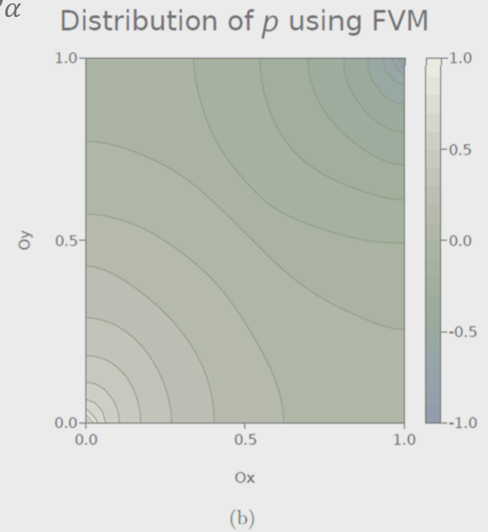
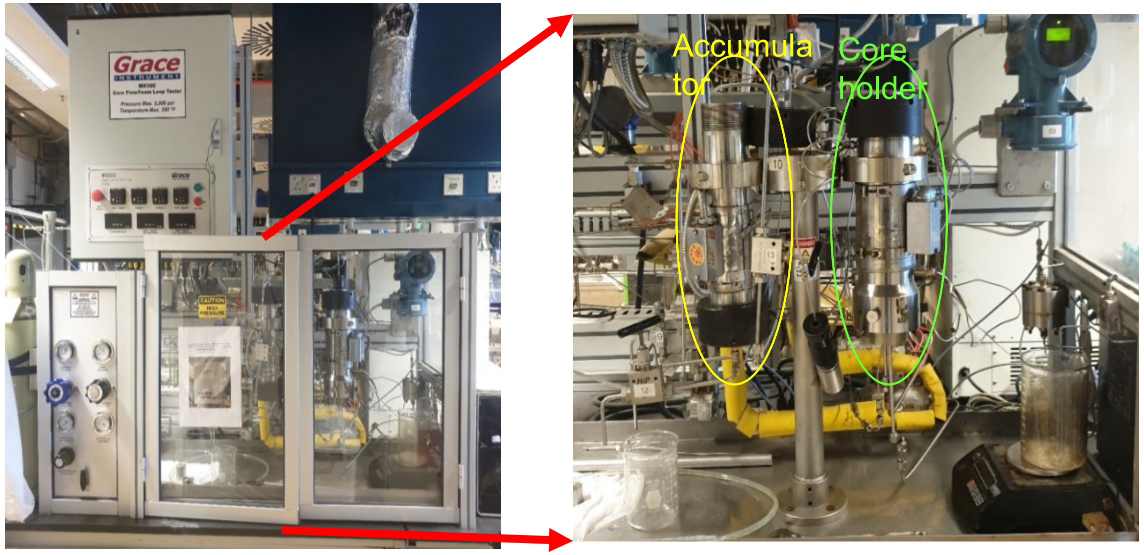
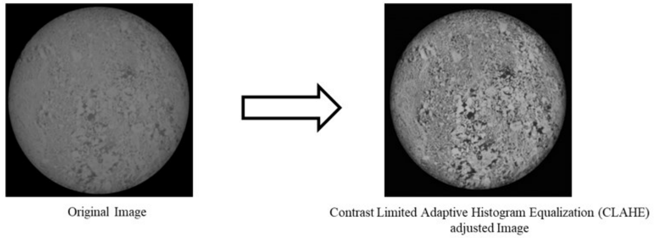


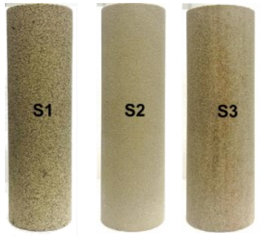


Experimental Investigations



The Core FlowLoop Tester instrument (left) and the accumulator and core holder within the closed chamber of the instrument (right) (Grace Instruments).





Experimental Investigations – CCS

Subsurface rock property extraction

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1. Micro Xray CT scan of the core samples from reservoirs analogous to Lithuanian reservoir.
2. Image pre-processing to improve the quality of scanned images.
3. Segmentation using k-means algorithm to determine porosity.
4. Lattice Boltzmann flow simulation to determine permeability.
5. Porosity and permeability estimation on sub-volumes to determine the representative element volume (REV).

Experimental Investigations – CCS

Laboratory measurements

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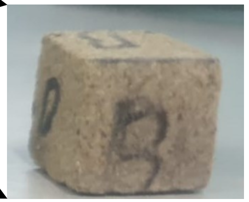
- Scanning of the core samples: Micro Xray-Computed Tomography (MXCT) scans were obtained using Skyscan 1275 © Bruker.
- Scanning resolution: The samples are scanned at two different resolutions, low resolution (22um) and high resolution (8um).

Instrument used for scanning core samples

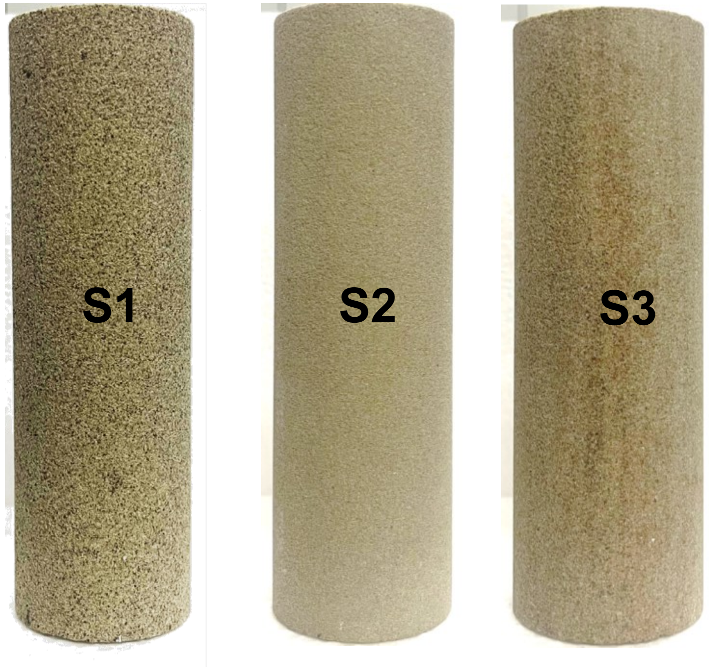
Core sample for low resolution scanning (22um)



Cube extracted for high resolution scanning (8um)

Research Topic Highlights – CCS (Subsurface Storage Investigations)

- In this study, sandstone samples are used, primarily composed of quartz as the dominant mineralogy with minor occurrences of clay minerals.



Sample name	Porosity (%)	Permeability (mD)
S1	21.60	275
S2	19.90	62
S3	20.22	327

Research Topic Highlights – CCS (Subsurface Storage Investigations)

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Sample Sets

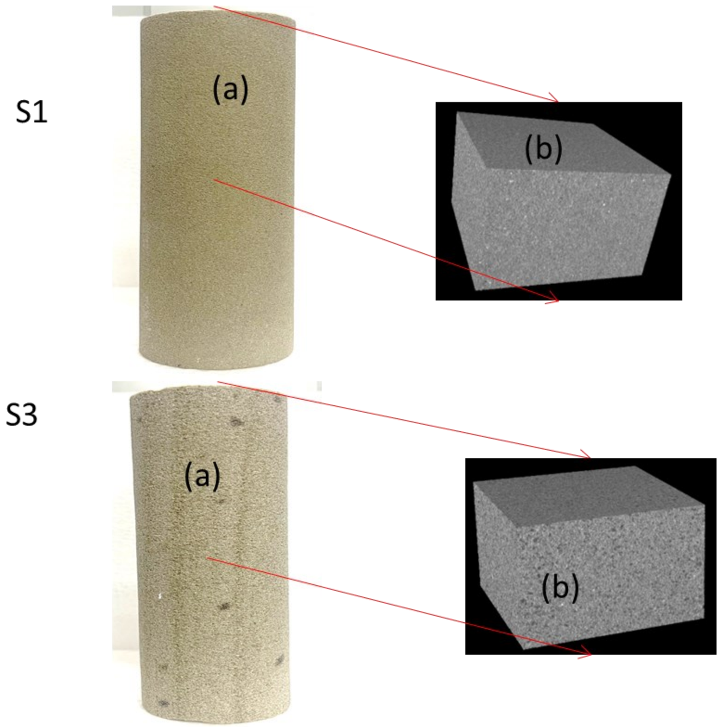
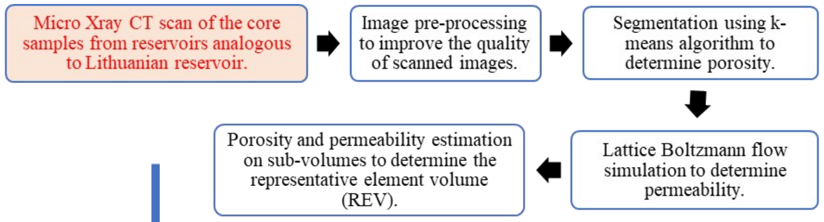


Figure: (a) A core sample with length = 2.5inch and diameter = 1.5inch and, (b) raw 3D volume generated from MXCT imaging at resolution of 22um. The 3D volume size is 941 X 941 X 601 pixels.



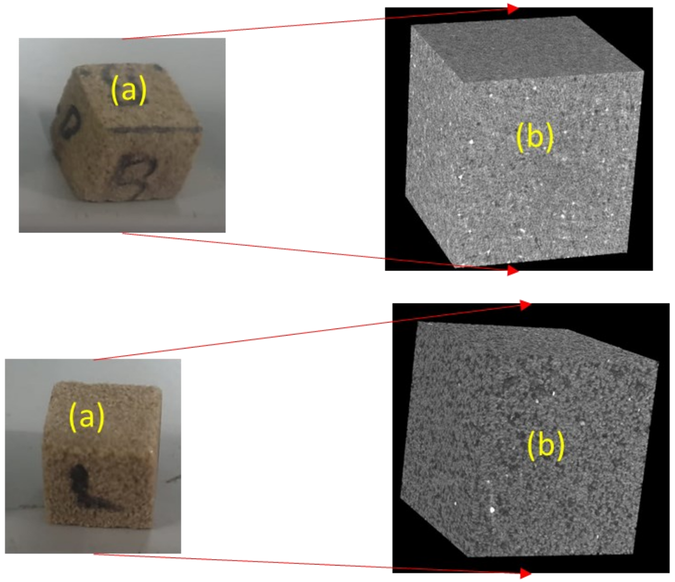
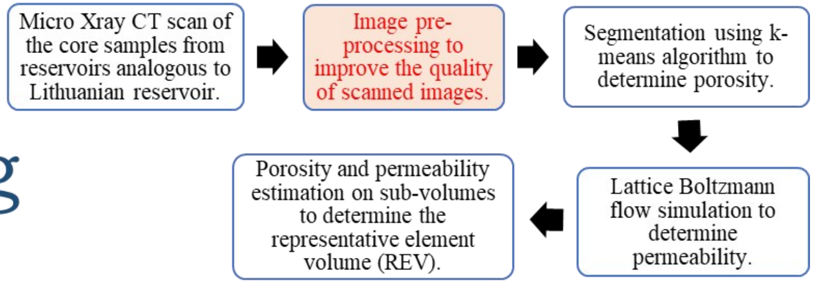
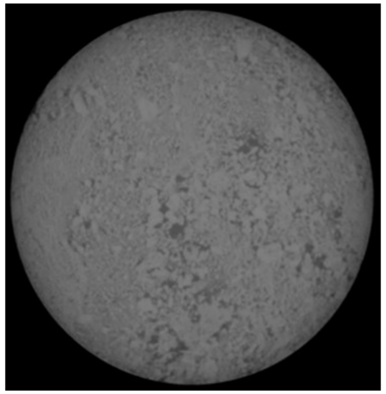


Figure: (a) A sample cube of 2cm, (b) raw 3D volume generated from MXCT imaging at resolution of 8um. The 3D volume size is 1020 X 1020 X 1014 pixels.

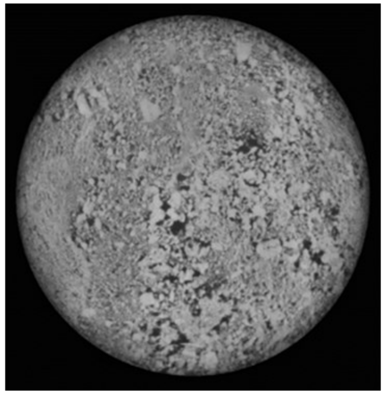
Research Topic Highlights – CCS (Subsurface Storage Investigations)



Results: Image Pre-processing



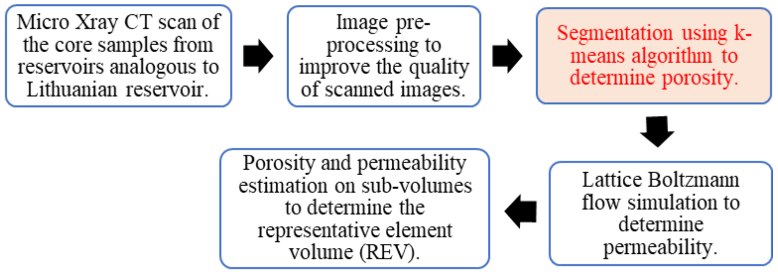
Original Image

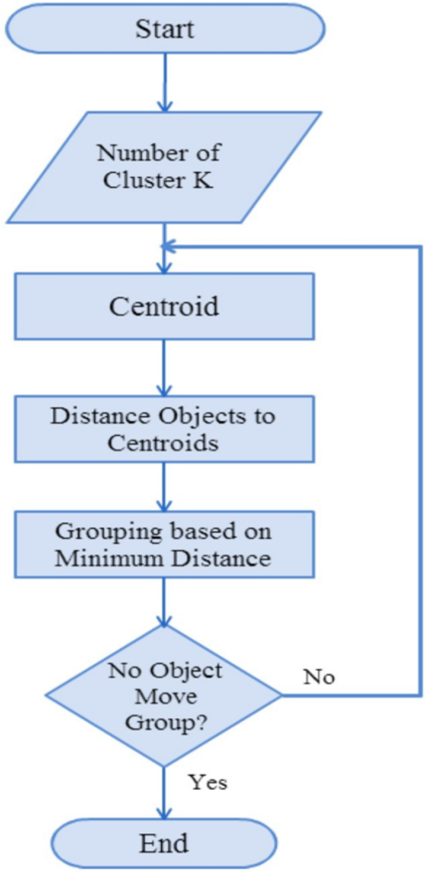


Contrast Limited Adaptive Histogram Equalization (CLAHE) adjusted Image

Research Topic Highlights – CCS (Subsurface Storage Investigations)

Segmentation: K-Means Algorithm





The objective function that is minimized is given by:

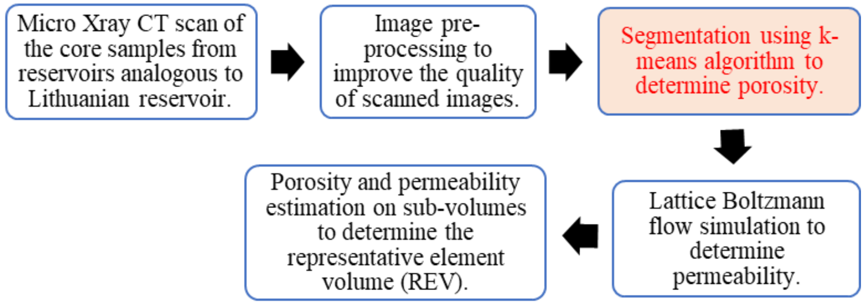
$$Z = \sum_{i=1}^{n} \sum_{j=1}^{k} \|x^{(i)} - C_j\|^2$$

Where, $\|x^{(i)} - C_j\|^2$ is the Euclidean distance between the data point x(i) and cluster centroid Cj.

$$C_j = \frac{1}{n} \sum_{i=1}^{n} x_j^{(i)}$$

Where n is the number of data points in the jth cluster and $x_j^{(i)}$ is the ith data point.

Research Topic Highlights – CCS (Subsurface Storage Investigations)



Results

Sample	Porosity using K-means algorithm (%)	Laboratory measured porosity (%)	Error (%)
S1	19.98	21.6	7.5
S2	19.70	19.9	1.0
S3	19.99	20.22	1.1

Table: Benchmarking of the porosity values with laboratory measured values

Research Topic Highlights – CCS (Subsurface Storage Investigations)

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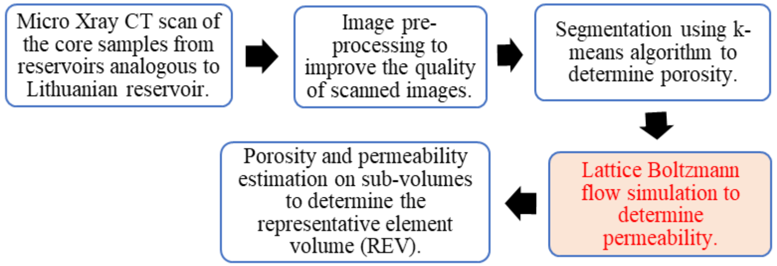
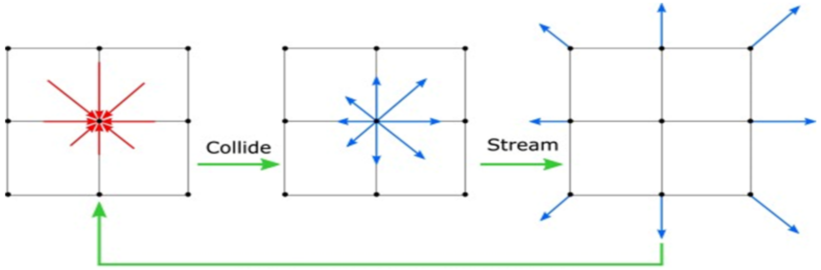
Lattice Boltzmann Method



- In the LBM, fluid is considered as a collection of particles that are represented by a probability distribution function at each discrete lattice node. The Lattice Boltzmann equation updates the probability distribution function at each time step and from this the velocities are calculated.
- LBM has 2 main steps: collision and streaming

Collision: $\tilde{f}_\alpha(\vec{x},t) = f_\alpha(\vec{x},t) - \frac{1}{\tau}\cdot\left(f_\alpha(\vec{x},t) - f^{eq}{}_\alpha(\vec{x},t)\right)$

Streaming: $f_\alpha(\vec{x} + \vec{v_\alpha}\cdot\Delta t, t + \Delta t) = \tilde{f}_\alpha(\vec{x},t)$



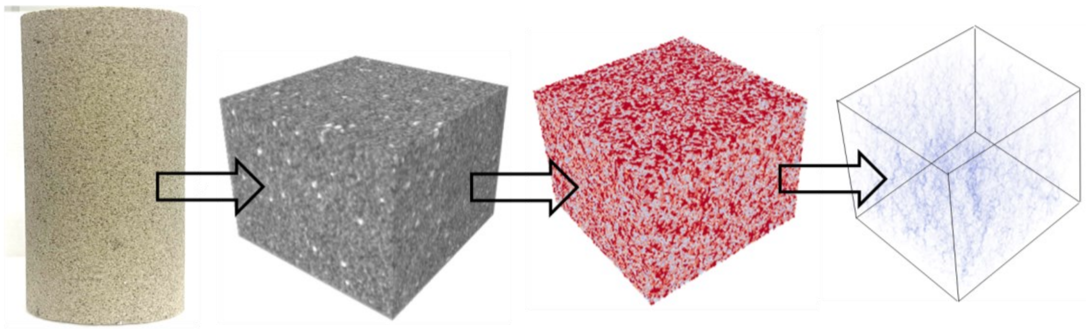
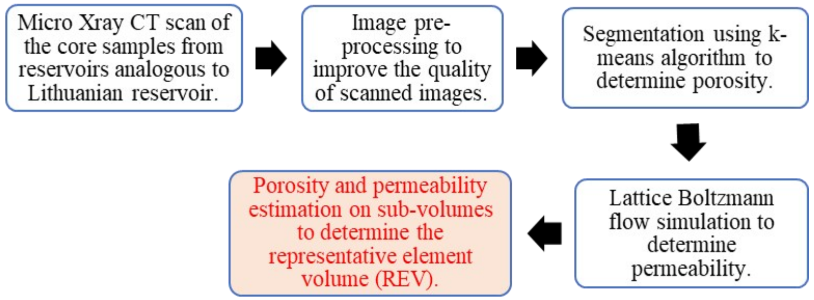


Figure: From left to right: Raw core sample, Scanned 3D volume, its segmented 3D volume and LBM simulated output, where blue thread like distribution shows the fluid flow through the pore space.

Research Topic Highlights – CCS (Subsurface Storage Investigations)

Results: Extraction of Sub-Volumes



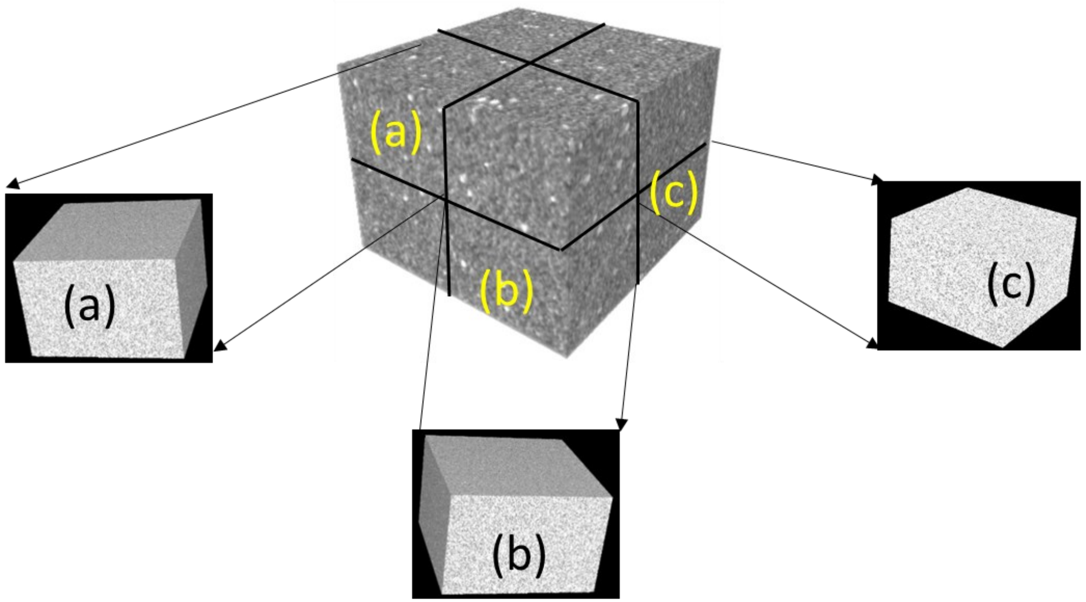


Figure: Illustration of the sub-volume extraction for fluid flow simulation

Results: Permeability estimation on sub-volumes using LBM simulation.

Sample	Sub-volumes	Permeability using LBM (mD)	Average permeability (mD)	Laboratory (mD)	Error (%)
S1	1	282	317	275	15
	2	307			
	3	360			
	4	320			
S2	1	83	91	62	47
	2	105			
	3	100			
	4	77			
S3	1	445	370	327	13
	2	334			
	3	370			
	4	330			

Research Topic Highlights – CCS (Subsurface Storage Investigations)

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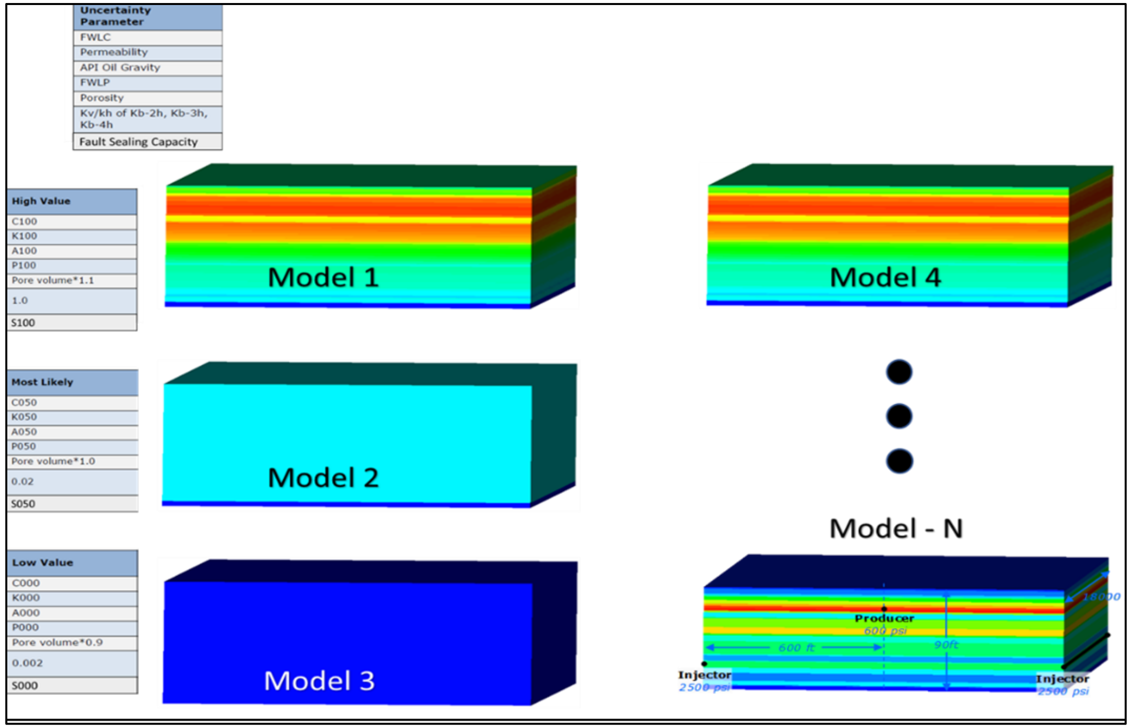
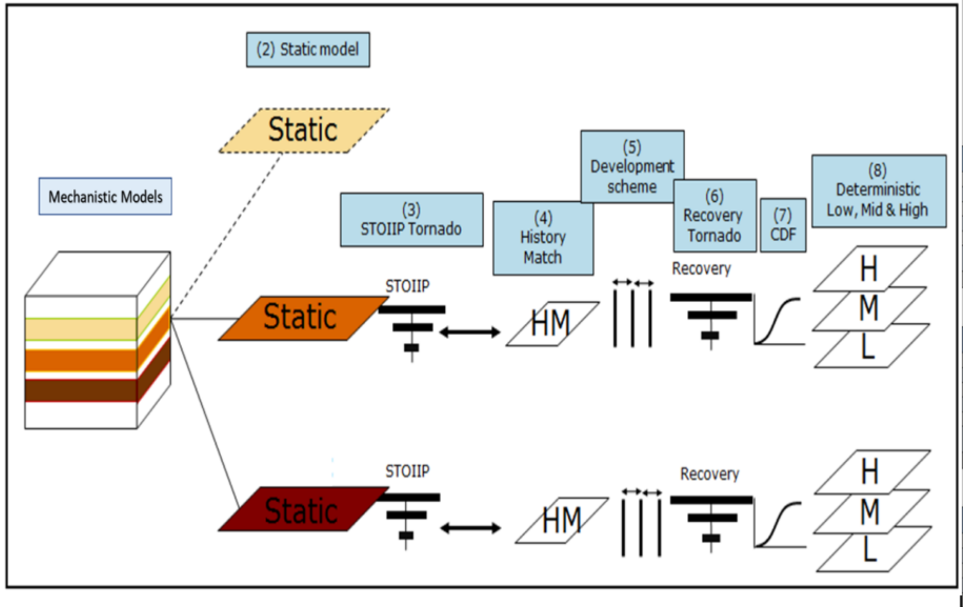
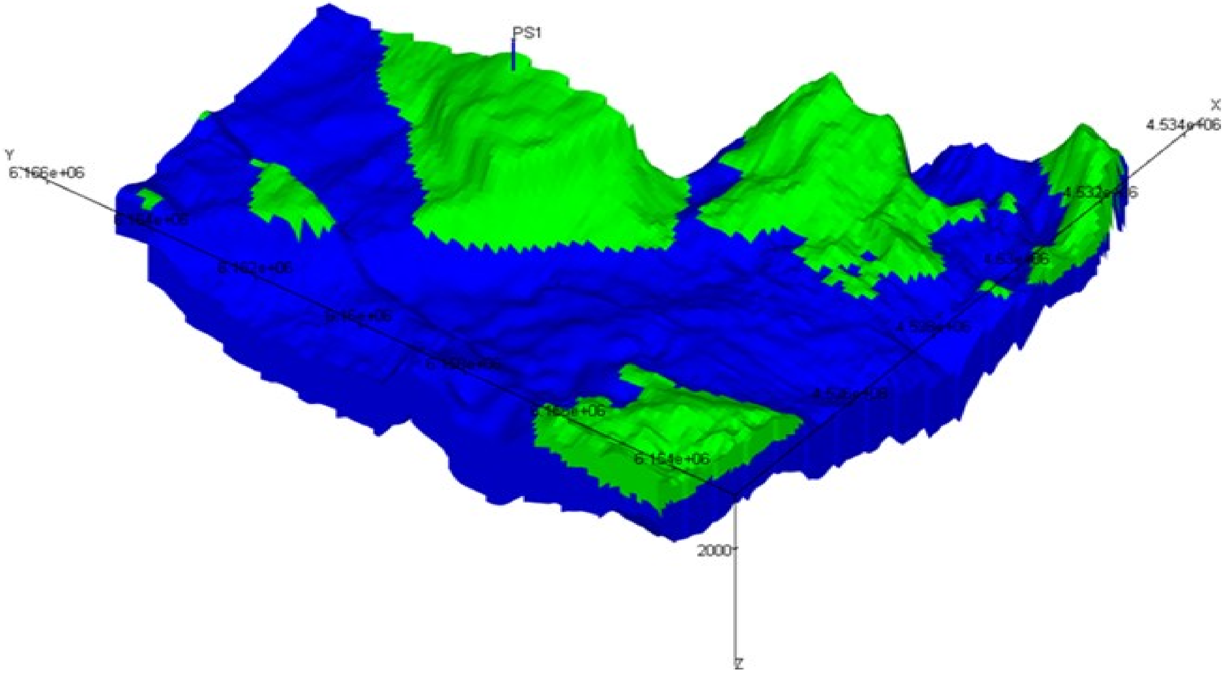
Re-evaluation methodology





Based on Principles of Uncertainty (probabilistic Modelling)
+ Thermodynamics and Phase Behavior

Research Topic Highlights – CCS (Subsurface Storage Investigations)



Gargzdai Oil Zone			
	Low	**Mid**	**High**
CO_2 (Mt)	64	94	267

Syderiai					D11				Vaskai		
	Low	**Mid**	**High**		**Low**	**Mid**	**High**		**Low**	**Mid**	**High**
CO_2 (Mt)	54	80	232		17	25	69		25	37	106

CCS: Summary

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- The present work provides a comprehensive analysis of CO_2 storage feasibility in Lithuanian formations.
- The present work can be further extended to provide a coupled geo-mechanical and geochemical impact on the injection and long-term storage integrity of CO_2.
- The present study focuses on interactions at the core scale, whereas interactions primarily occur at the pore scale.
- To examine the changes occurring at the pore scale, future work will include studying microfluidic interactions, which will further enhance the understanding of Lithuanian reservoirs.

Thanks