

CCS-Analytics

Carbon Capture and Storage using Science & Engineering
Application of Artificial Intelligence (SEA-AI)

Shahab Mohaghegh
West Virginia University

U.S. Department of Energy
National Energy Technology Laboratory
Carbon Management Project Review Meeting
August 15 - 19, 2022

Project Overview

- **Science & Engineering Application of AI (SEA-AI)**
 - Artificial Intelligence & Machine Learning (AI&ML)
 - AI-Ethics
 - Modeling Physics using AI&ML
 - Engineering Applications of AI&ML
- **Smart Proxy Modeling**
- **Engineering Case Study of SEA-AI**
 - Carbon Storage using SEA-AI

Artificial Intelligence & Machine Learning

Artificial Intelligence



The Technology that **Simulates Human Intelligence by Mimicking Human Brain** for Analysis, Modeling, and Decision Making

Machine Learning



The science of making computers to act
(a) without being explicitly programmed
(b) through using **Open Computer Algorithms and Learning from Data**

Machine Learning Algorithms

- Machine Learning Algorithms used for SEA-AI:
 - Artificial Neural Networks
 - Fuzzy Set Theory
 - Genetic Algorithm

AI+ML ALGORITHMS

Artificial Neural Networks

Fuzzy Set Theory

Genetic Algorithm

MIMICKING LIFE AND NATURE

Human Brain's Information Processing

Human Brain's logic

Optimization through Natural Selection

AI-Ethics

- Ethics of Artificial Intelligence became a research topic due to the creation of **Racism and Sexism** using AI in the past decade.
- Companies such as IBM, Google, Amazon, etc. that **unintentionally** developed the **racism and sexism** using AI-models have made efforts to research and address biases in AI-models.
- One solution for addressing bias is to create documentation for the data used to train the AI systems.

MIT Technology Review of AI-Ethics

“The problem of **bias** in machine learning is likely to become more significant as the technology spreads to critical areas like medicine and law (**and engineering**), and as more people without a **deep technical understanding** are tasked with deploying it.

Some experts warn that algorithmic **bias is already pervasive in many industries** and that almost **no one is making an effort to identify or correct it**”.

AI-Ethics in Engineering

- “AI-based Modeling of Physics” is purely based on **Fact** and **Reality** through “Actual Measurements”.
- “Traditional Physics-based Modeling” includes some of the following items through “Mathematical Equations”.
 - **Assumptions, Interpretations, Simplifications, Preconceived Notions, and Biases.**
- By including data from “Mathematical Equations” to “Actual Measurements” *You Are Telling AI-based Model* **“What To Do”**.

Proxy Modeling

- Proxy Model is a **mathematically** or **statistically** defined function that replicates or approximates the response of the full-scale simulation model output for selected input parameters.

Denney 2010

- Since deployment of the “**full-scale simulation model**” of complex physical phenomena takes a long time even on HPC, the objective of the Proxy Model is to perform numerical simulation in a very short time period.

Proxy Modeling

- Currently, there are two types of Proxy Models for Numerical Simulations:
 - **Traditional Proxy Models:**
 - Generating the Proxy Models using mathematical or statistical approaches.
 - **Smart Proxy Model:**
 - Generating the Proxy Models using Artificial Intelligence & Machine Learning approach.

Smart Proxy Modeling

- Smart Proxy Modeling is **teaching** engineering problem solving to an **open computer algorithm** using **data from numerical simulation**
 - **Data from Numerical Simulation** includes:
 - Data that is used to build the numerical simulation
 - Feature generation that explains (teaches to the machine learning algorithm) the ***physics and numerical solution*** of the numerical simulation
- It is impossible to do this** if you are not a Domain Expert in the development of the numerical simulation

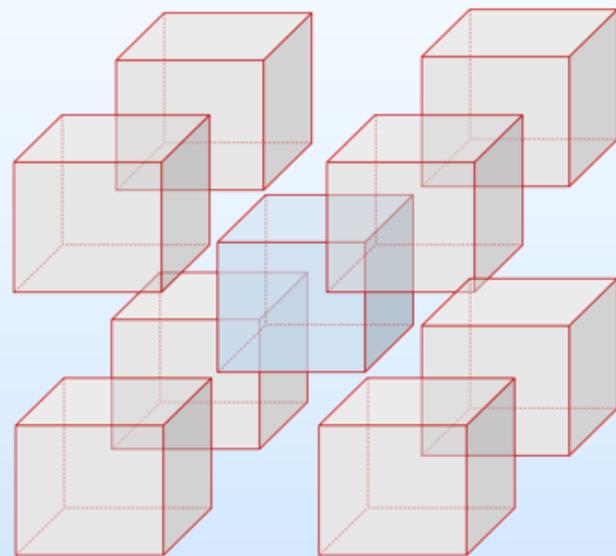
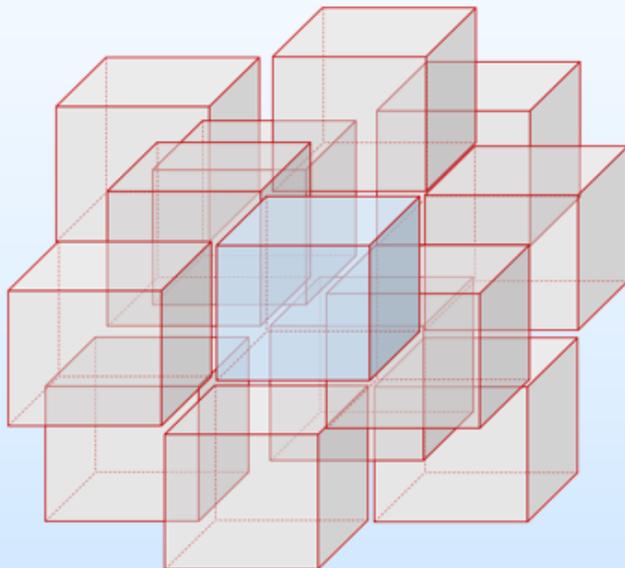
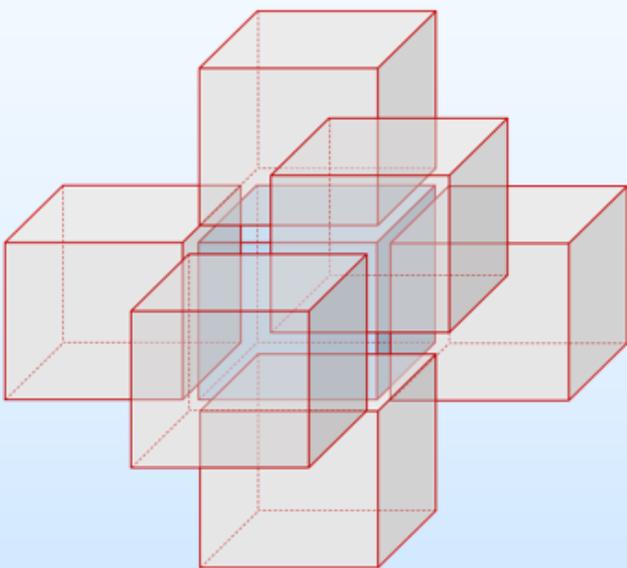
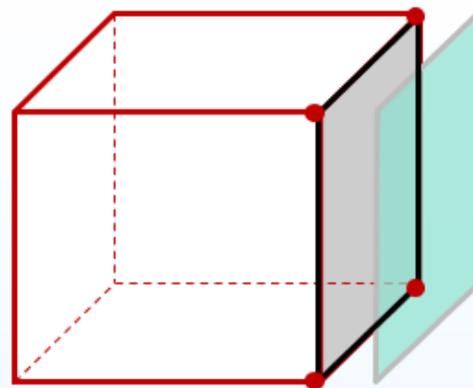
Smart Proxy Modeling

- Smart Proxy Modeling lets the Numerical Simulation easily be used for important characteristics:
 - Reservoir Pressure and CO₂ Saturation distribution in Space and Time for every cell in the Numerical Simulation
 - History Matching
 - Uncertainty Quantification
 - CO₂ Injection Optimization
 - CO₂ Leakage Detection
 - ...

Smart Proxy Modeling

- Smart Proxy Model Development for Numerical Simulation requires:
 - Unlike Traditional Statistics that require hundreds of numerical simulation runs to generate Proxy Model, AI-based Proxy Model (Smart Proxy Model) only requires around 20 numerical simulation runs.

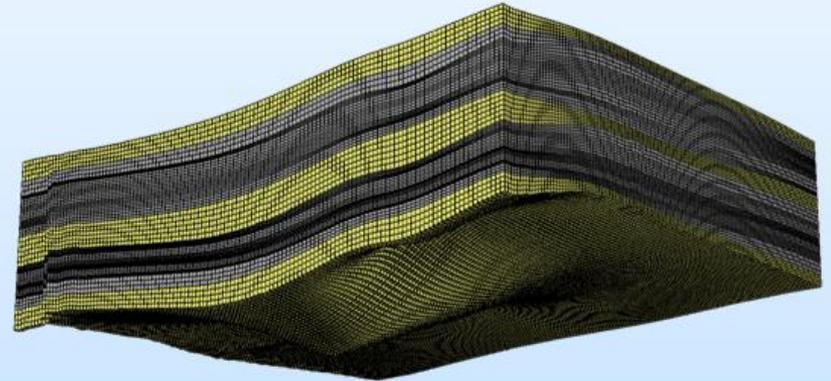
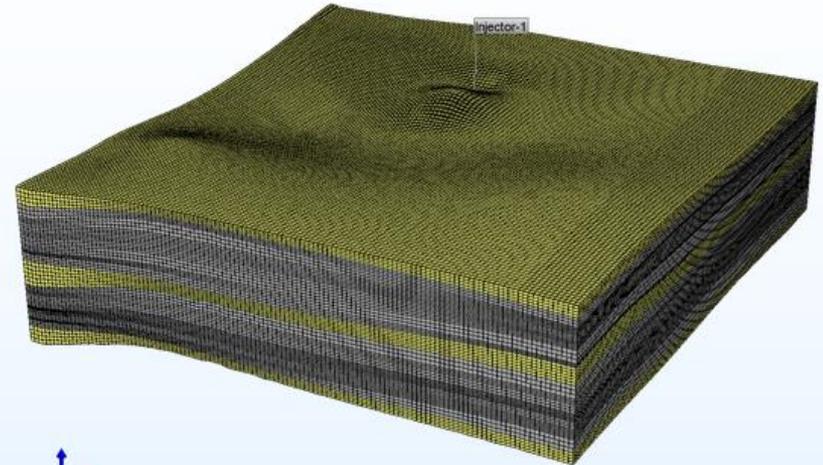
Smart Proxy Model Development



Case Study

CO₂ Storage in Saline Aquifer Numerical Reservoir Simulation

- Heterogeneous Reservoir Characteristics
 - Various Layer Thicknesses
 - Layers are not flat
 - Grid blocks are not the same size
- Saline Aquifer formations (Sands)
- Cap Rocks (Shale)

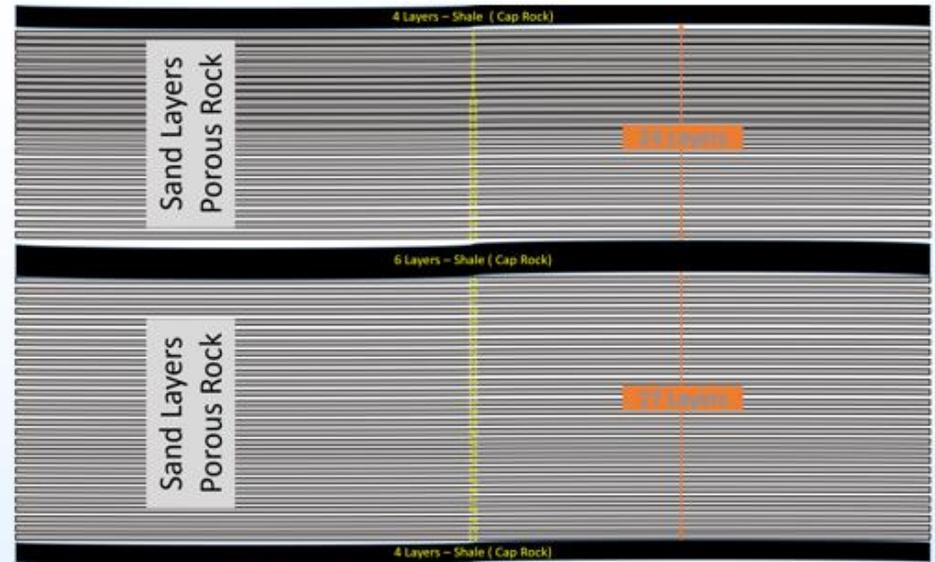


CO₂ Storage in Saline Aquifer

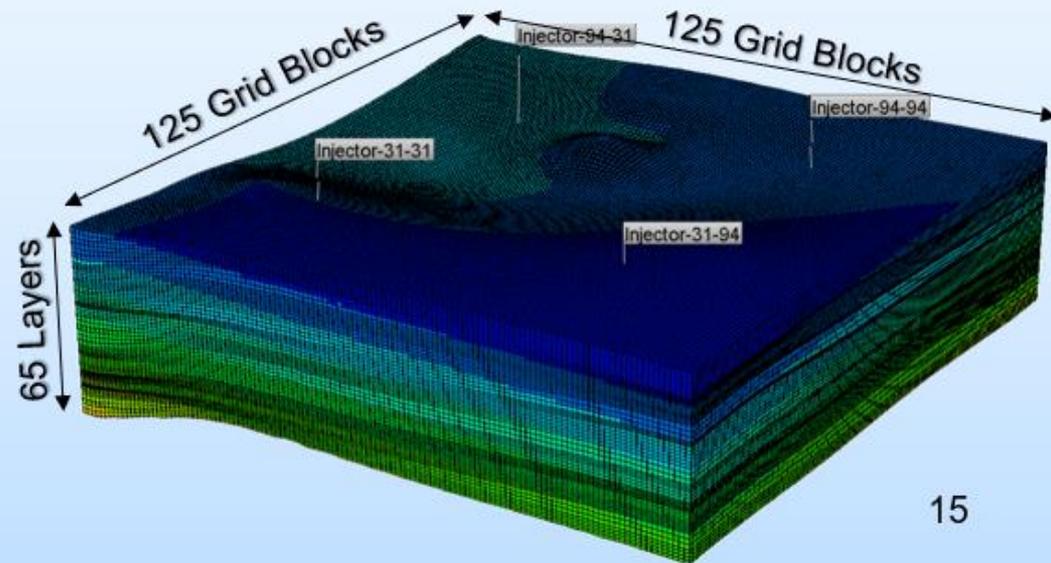
Grid Blocks

$$125 \times 125 \times 61 = 1,015,625$$

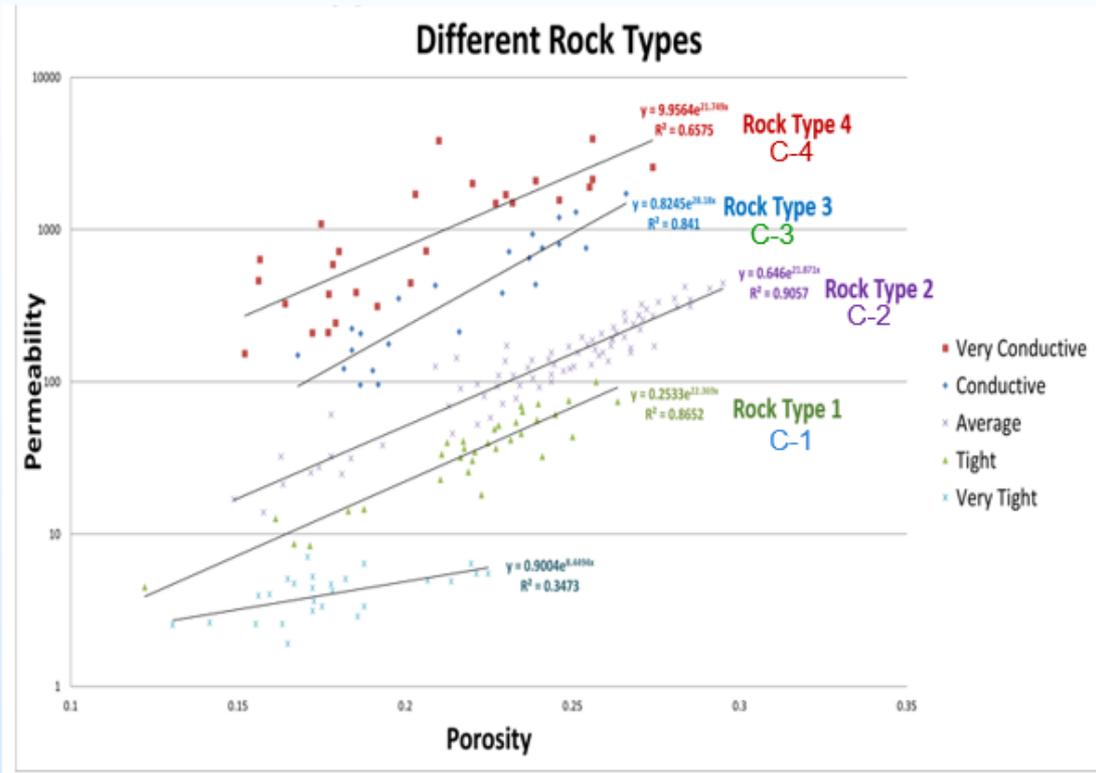
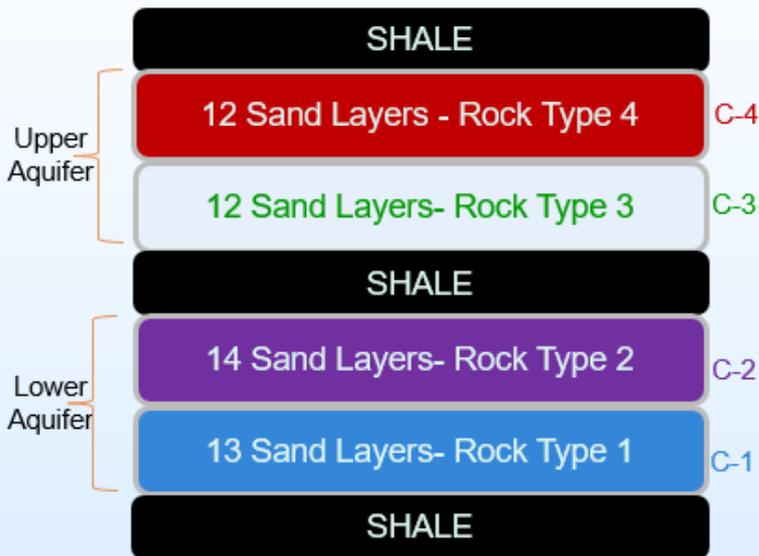
CO₂ is Stored through
4 Injection wells



Some of reservoir data are taken from Citronelle field, a saline reservoir located in Mobile County (Alabama, US)



CO₂ Storage in Saline Aquifer



CO₂ Storage in Saline Aquifer

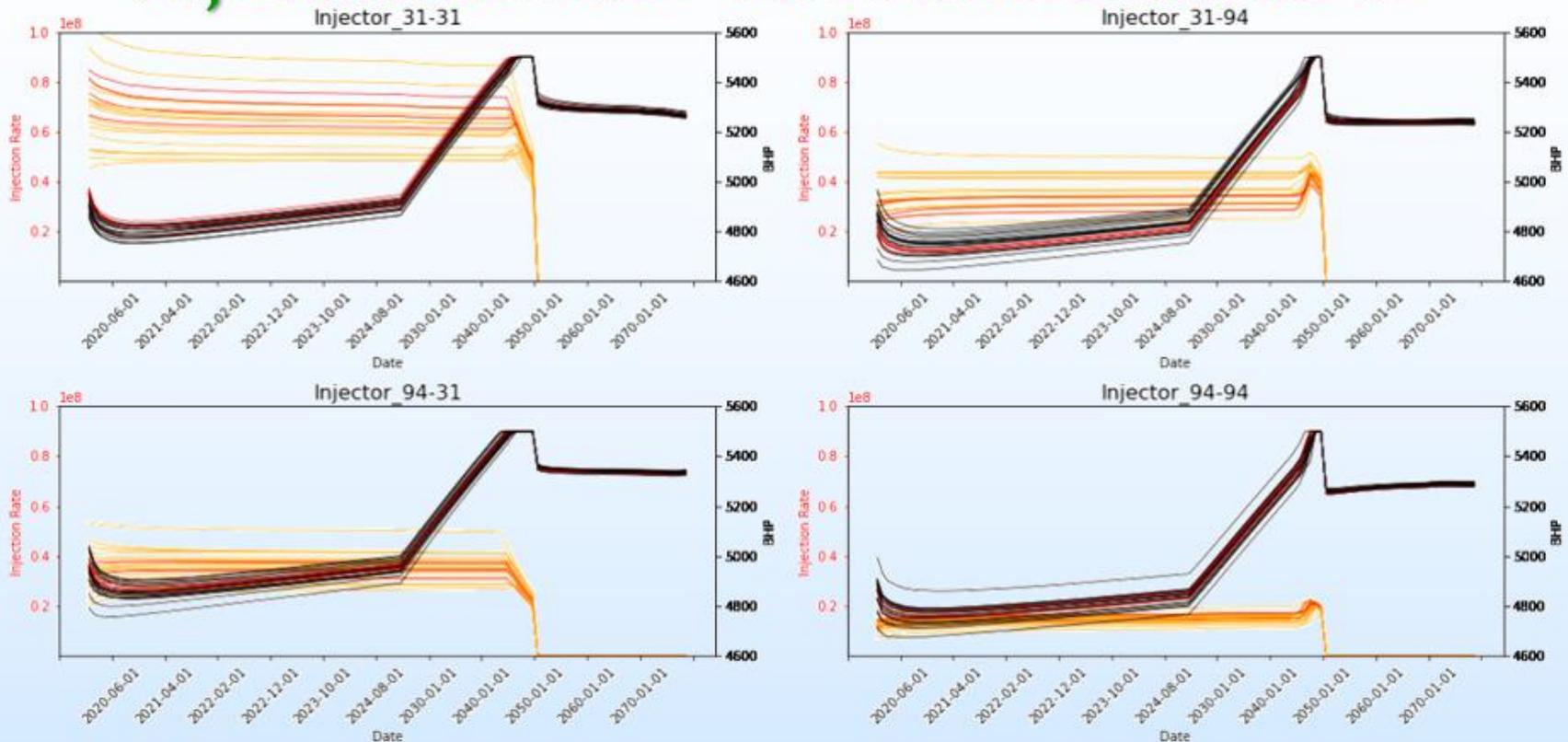
CO₂ Injection Design

- Four CO₂ injector wells
- The injector wells are completed in all 51 sand layers
- The Injectors well will be operating using two constraints.
 - Bottom Hole Pressure
 - Max Injection Rate



CO₂ Storage in Saline Aquifer

Injection and BHP for 20 Simulation Runs



300 Years of Numerical Reservoir Simulation Model

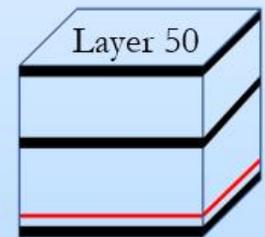
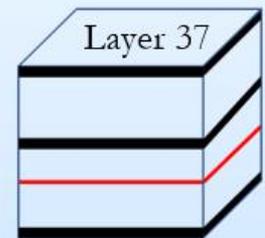
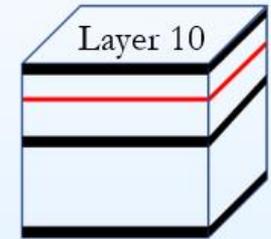
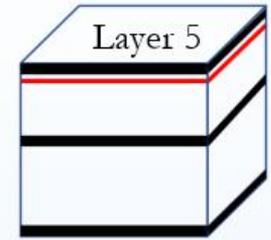
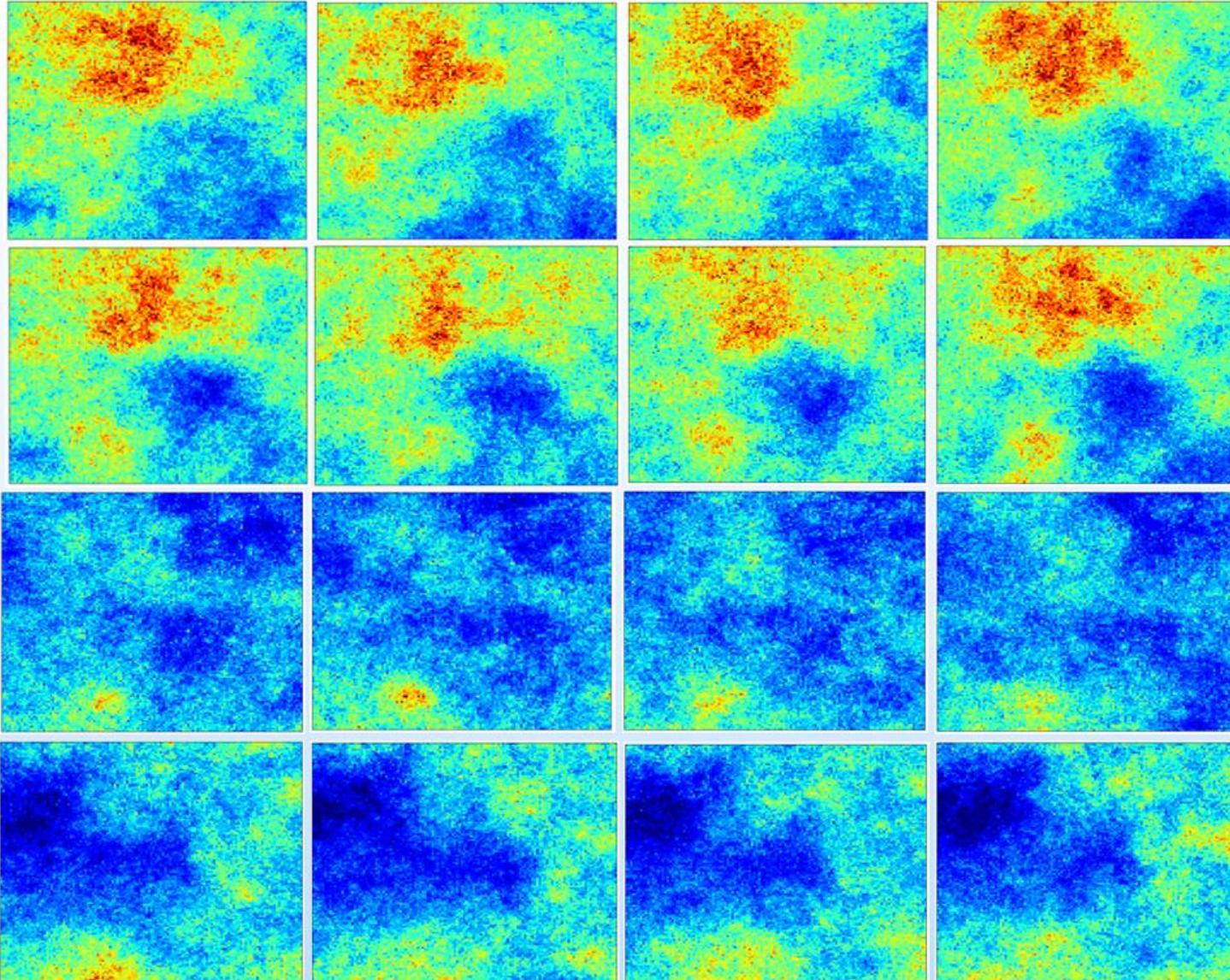
20 Geological Realizations

Geological Realization #1

Geological Realization #4

Geological Realization #10

Geological Realization #20



CO₂ Storage in Saline Aquifer

Data Used for Smart Proxy
Model Development

Smart Proxy Model Development
includes Training (80%),
Calibration (10%), and Validation (10%)

Data Used for Smart Proxy
Blind Validation

Data for Blind Validation
is NOT used during
Smart Proxy Model Development

Geological Realization #1

Geological Realization #2

Geological Realization #3

Geological Realization #4

Geological Realization #5
Simulation Run 05

Geological Realization #6

Geological Realization #7

Geological Realization #8

Geological Realization #9
Simulation Run 09

Geological Realization #10

Geological Realization #11

Geological Realization #12

Geological Realization #13
Simulation Run 13

Geological Realization #14

Geological Realization #15

Geological Realization #16

Geological Realization #17
Simulation Run 17

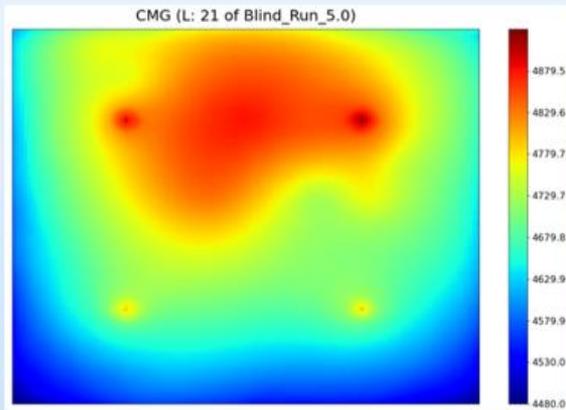
Geological Realization #18

Geological Realization #19

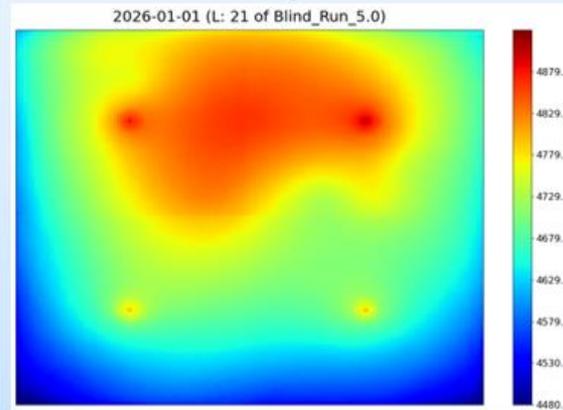
Geological Realization #20

Pressure Distribution at a Specific Time (January 2026) in a Layer (Layer 21) in a Specific Blind Validation Simulation Run (Blind Validation – Run #5)

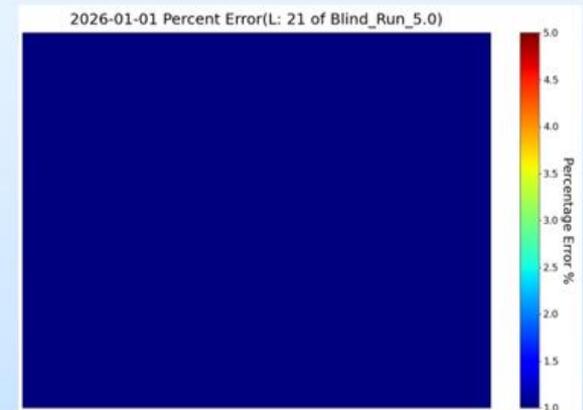
Commercial Numerical Reservoir
Simulation - CMG



AI-based Proxy Model
Smart Proxy Model



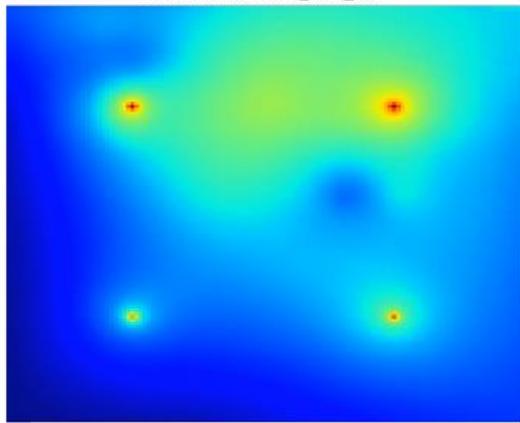
Accuracy of Smart Proxy Model
1% to 5% Error



BLIND RUN #5 – Time-Step Feb. 2020

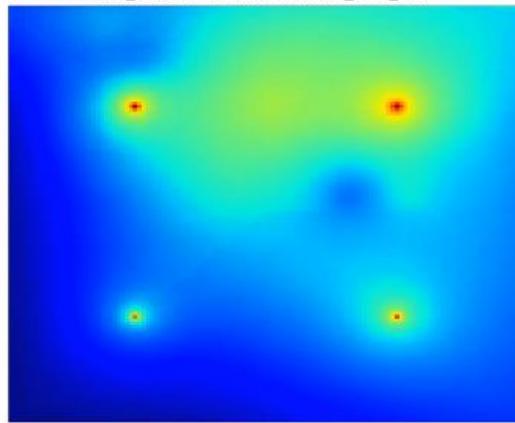
Reservoir Pressure
Distribution Video

CMG (L: 5 of Blind_RUN_05)



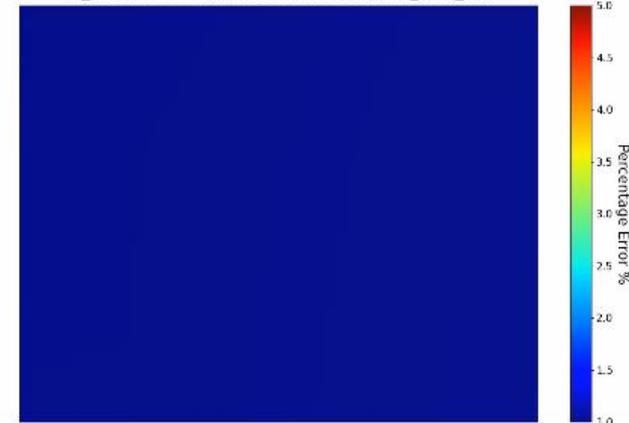
CMG - Numerical Reservoir Simulation

Pr_2020-02-01 (L: 5 of Blind_RUN_05)

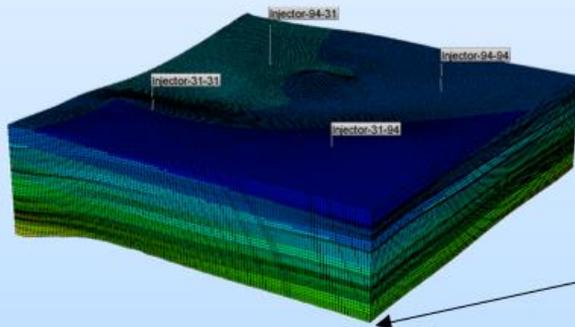


Smart Proxy Model

Pr_2020-02-01 Percent Error(L: 5 of Blind_RUN_05)



%Error

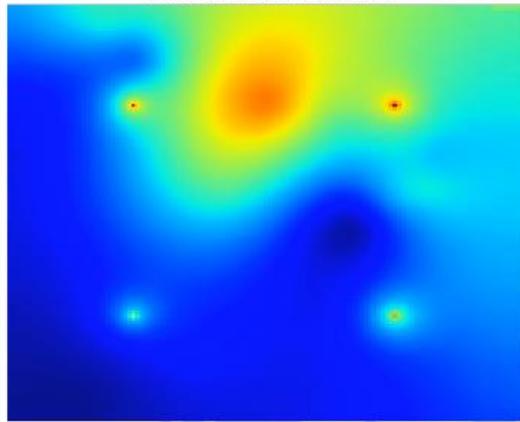


Reservoir Pressure value at every single cell (51 layers) at a certain Time-step

BLIND RUN #5 – Time-Step Feb. 2020

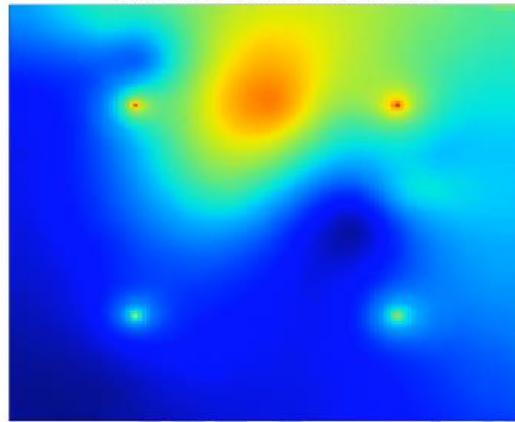
Reservoir Pressure
Distribution Video

CMG (L: 61 of Blind_RUN_05)



CMG - Numerical Reservoir Simulation

Pr_2020-02-01 (L: 61 of Blind_RUN_05)

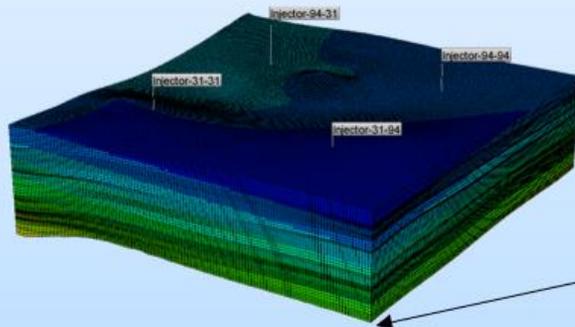


Smart Proxy Model

Pr_2020-02-01 Percent Error(L: 61 of Blind_RUN_05)



%Error



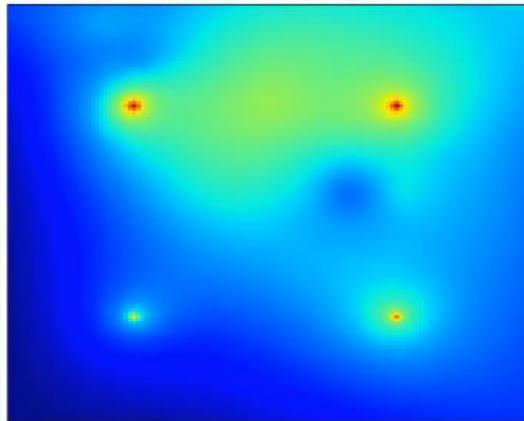
Reservoir Pressure value at every single cell (51 layers) at a certain Time-step

BLIND RUN #9 – Time-Step

Feb. 2020

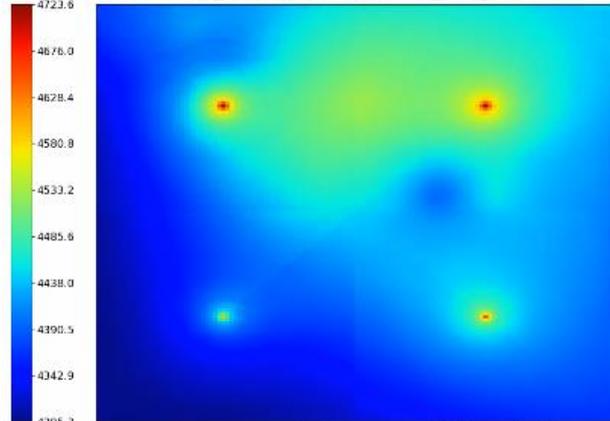
Reservoir Pressure Distribution Video

CMG (L: 5 of Blind_RUN_09)



CMG - Numerical Reservoir Simulation

Pr_2020-02-01 (L: 5 of Blind_RUN_09)

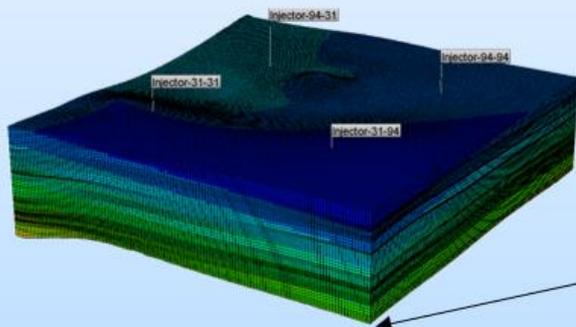


Smart Proxy Model

Pr_2020-02-01 Percent Error(L: 5 of Blind_RUN_09)



%Error



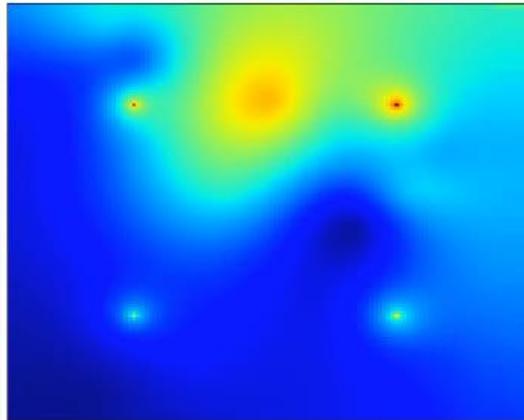
Reservoir Pressure value at every single cell (51 layers) at a certain Time-step

BLIND RUN #9 – Time-Step

Feb. 2020

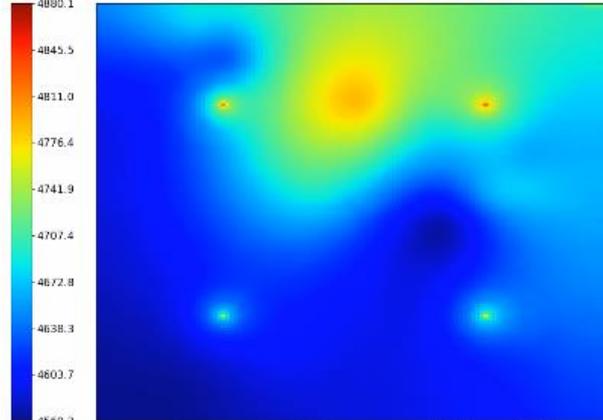
Reservoir Pressure
Distribution Video

CMG (L: 61 of Blind_RUN_09)



CMG - Numerical Reservoir Simulation

Pr_2020-02-01 (L: 61 of Blind_RUN_09)

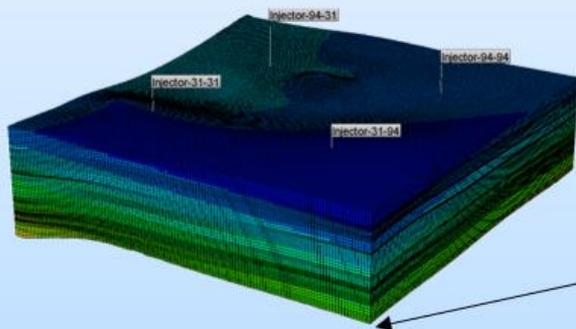


Smart Proxy Model

Pr_2020-02-01 Percent Error(L: 61 of Blind_RUN_09)



%Error



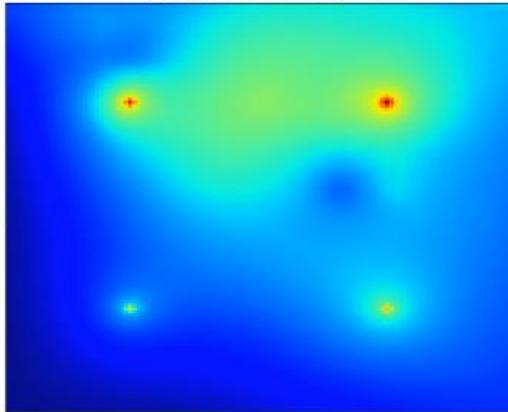
Reservoir Pressure value at every single cell (51 layers) at a certain Time-step

BLIND RUN #13 – Time-Step

Feb. 2020

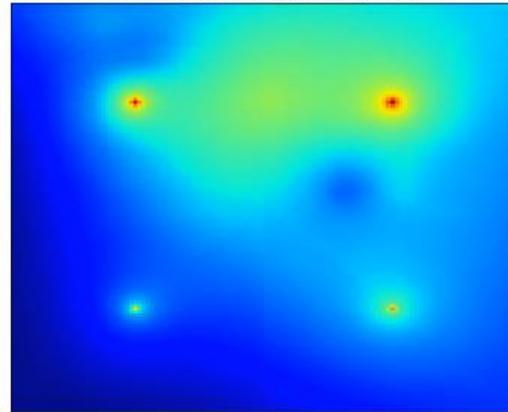
Reservoir Pressure
Distribution Video

CMG (L: 5 of Blind_RUN_13)



CMG - Numerical Reservoir Simulation

Pr_2020-02-01 (L: 5 of Blind_RUN_13)

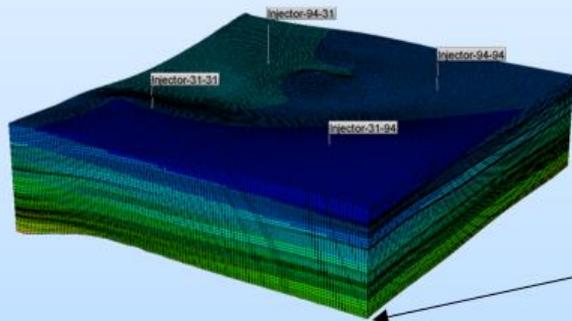


Smart Proxy Model

Pr_2020-02-01 Percent Error(L: 5 of Blind_RUN_13)



%Error



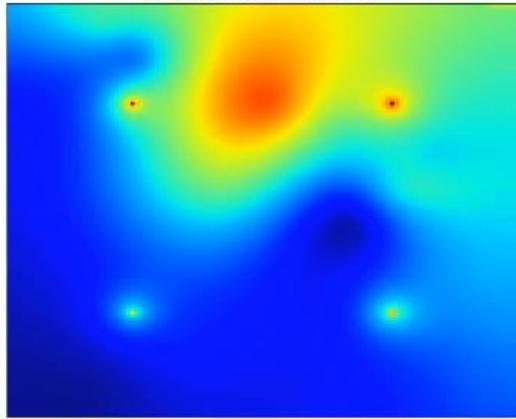
Reservoir Pressure value at every single cell (51 layers) at a certain Time-step

BLIND RUN #13 – Time-Step

Feb. 2020

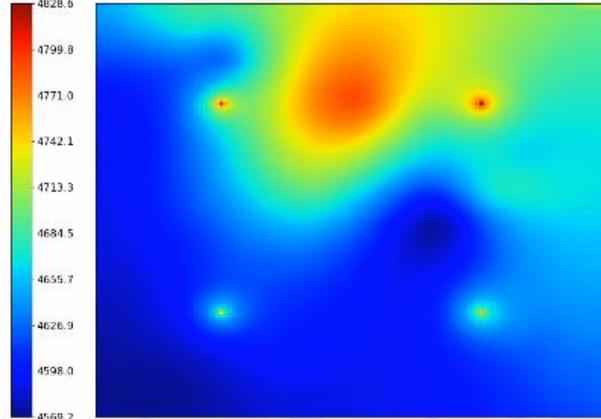
Reservoir Pressure
Distribution Video

CMG (L: 61 of Blind_RUN_13)



CMG - Numerical Reservoir Simulation

Pr_2020-02-01 (L: 61 of Blind_RUN_13)

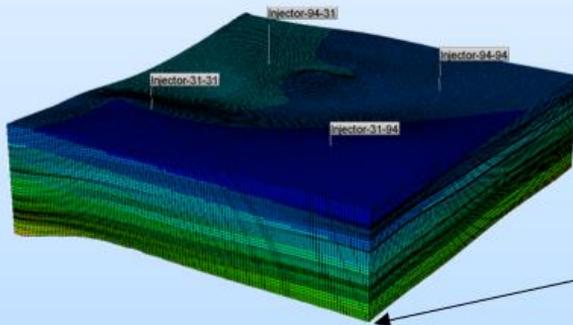


Smart Proxy Model

Pr_2020-02-01 Percent Error(L: 61 of Blind_RUN_13)



%Error



Reservoir Pressure value at every single cell (51 layers) at a certain Time-step

BLIND RUN #17 – Time-Step

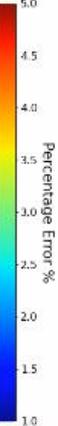
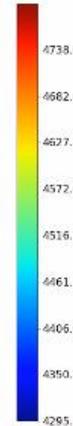
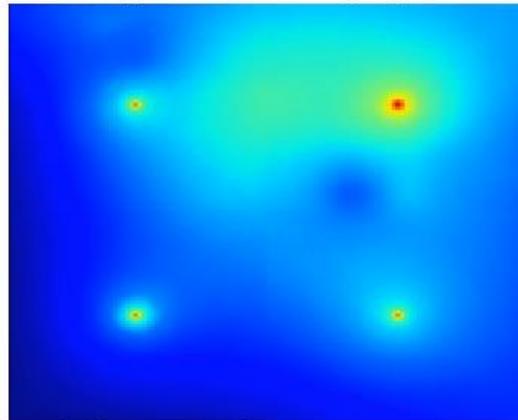
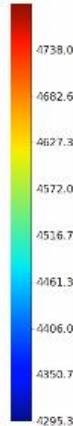
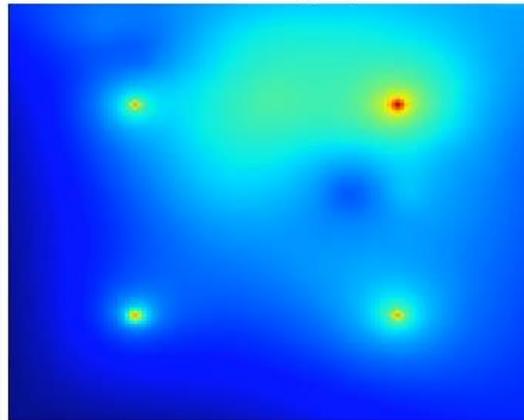
Reservoir Pressure
Distribution Video

Feb. 2020

CMG (L: 5 of Blind_RUN_17)

Pr_2020-02-01 (L: 5 of Blind_RUN_17)

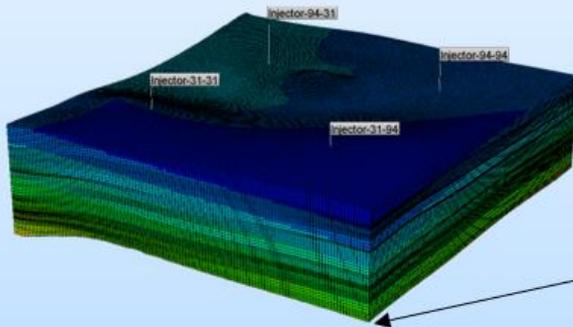
Pr_2020-02-01 Percent Error(L: 5 of Blind_RUN_17)



CMG - Numerical Reservoir Simulation

Smart Proxy Model

%Error



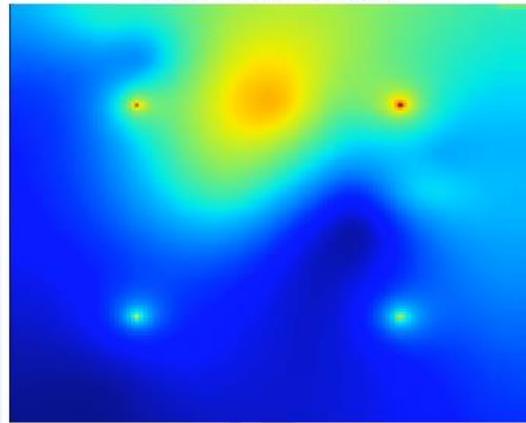
Reservoir Pressure value at every single cell (51 layers) at a certain Time-step

BLIND RUN #17 – Time-Step

Reservoir Pressure
Distribution Video

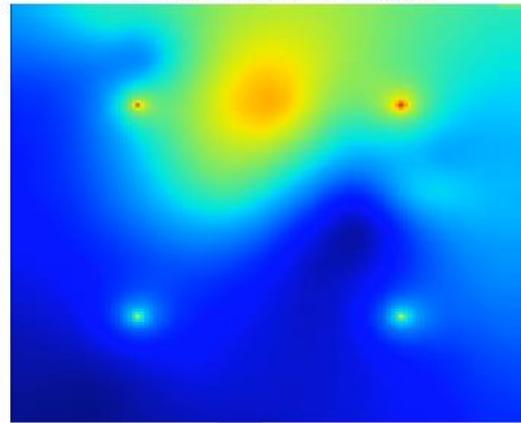
Feb. 2020

CMG (L: 58 of Blind_RUN_17)



CMG - Numerical Reservoir Simulation

Pr_2020-02-01 (L: 58 of Blind_RUN_17)

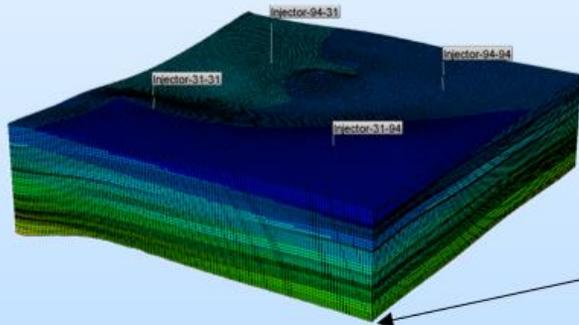


Smart Proxy Model

Pr_2020-02-01 Percent Error(L: 58 of Blind_RUN_17)



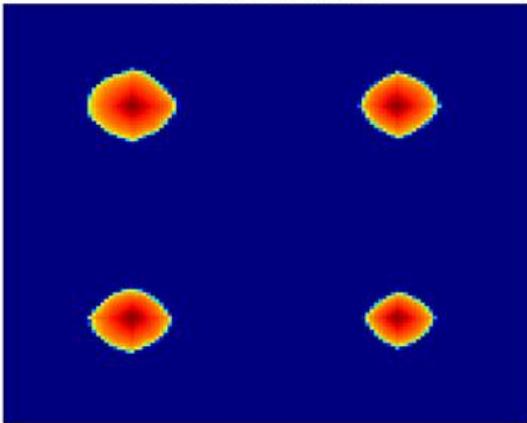
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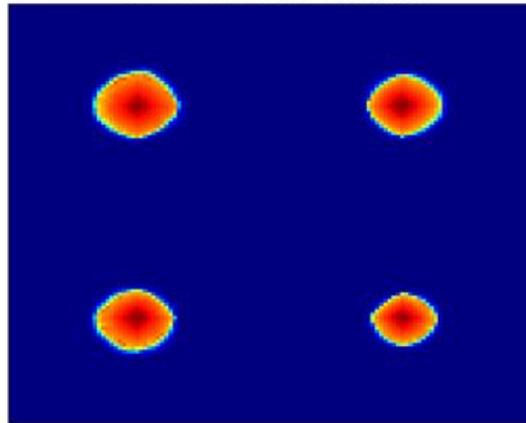
Reservoir Pressure value at every single cell (51 layers) at a certain Time-step

CO₂ Saturation Distribution Video

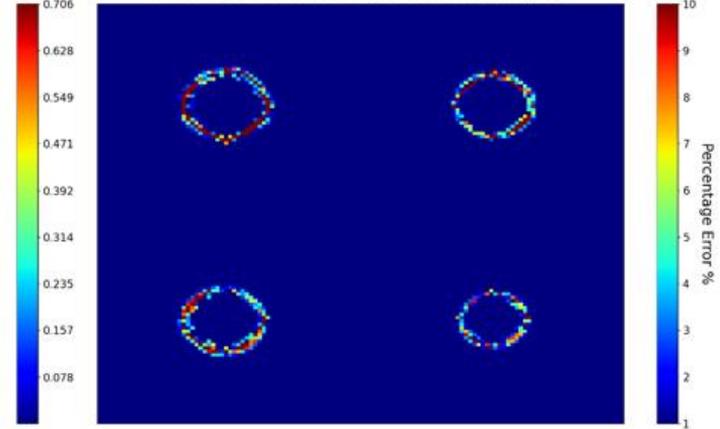
CMG (L: 06 of Blind_Run_5.0)



2023-01-01 (L: 06 of Blind_Run_5.0)



2023-01-01 Percent Error(L: 06 of Blind_Run_5.0)



CMG - Numerical Reservoir Simulation

Smart Proxy Model

%Error

January 2023



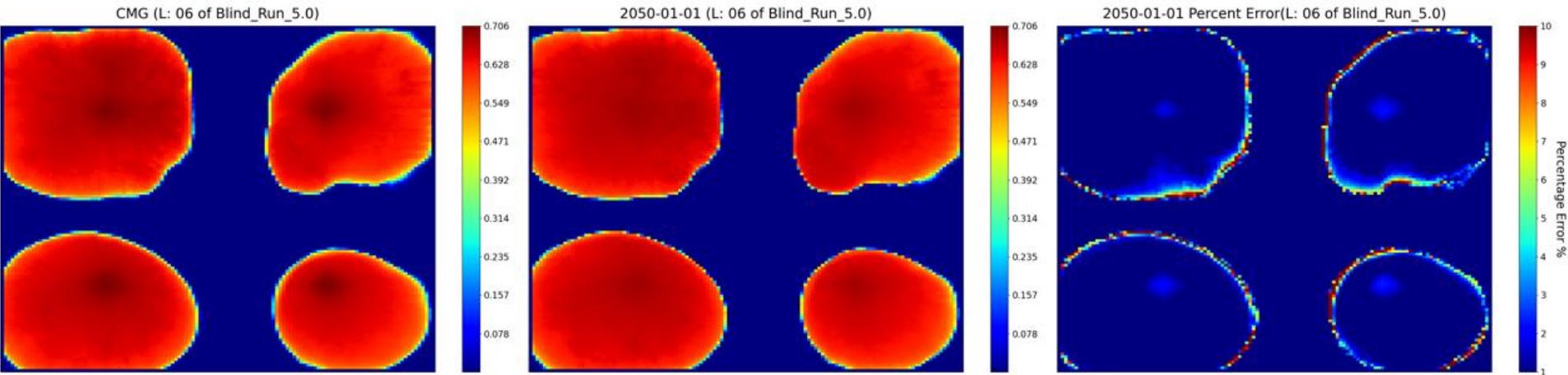
Annual Distribution
CO₂ Saturation

From: January 2023
To: January 2050

Blind Validation

Geological Realization #5, Layer 6

CO₂ Saturation Distribution Video



CMG - Numerical Reservoir Simulation

Smart Proxy Model

%Error

January 2050



Blind Validation

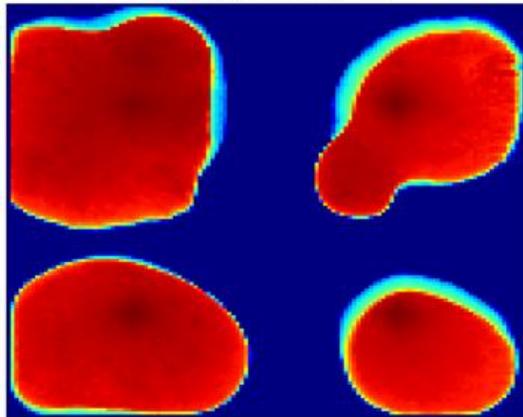
Geological Realization #5, Layer 6

**Annual Distribution
CO₂ Saturation**

**From: January 2023
To: January 2050**

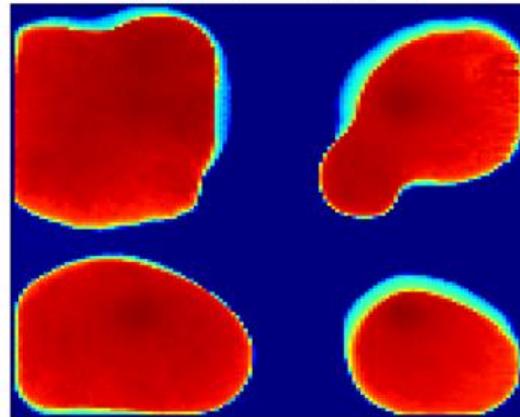
CO₂ Saturation Distribution Video

CMG (L: 07 of Blind_Run_5.0)



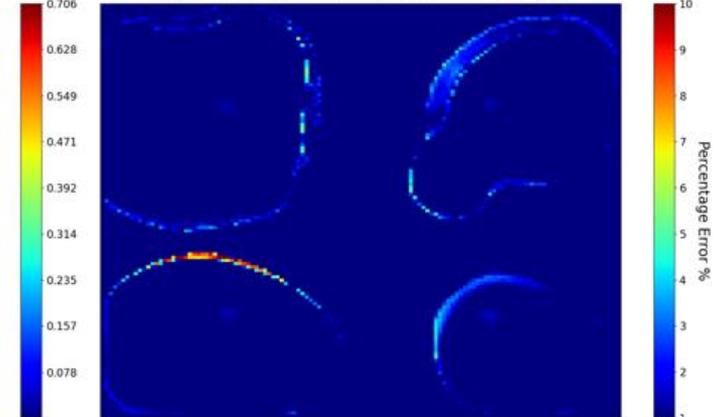
CMG - Numerical Reservoir Simulation

2070-01-01 (L: 07 of Blind_Run_5.0)



Smart Proxy Model

2070-01-01 Percent Error(L: 07 of Blind_Run_5.0)



%Error

January 2070



Blind Validation

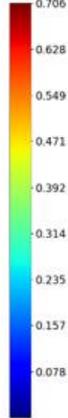
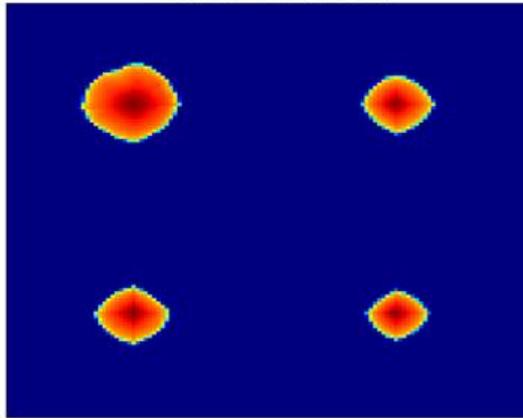
Geological Realization #5, Layer 7

Annual Distribution
CO₂ Saturation

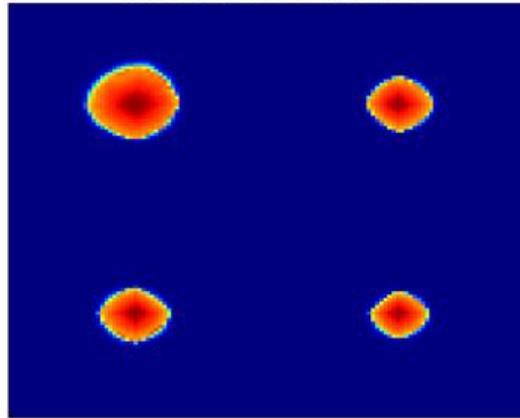
From: January 2051
To: January 2070

CO₂ Saturation Distribution Video

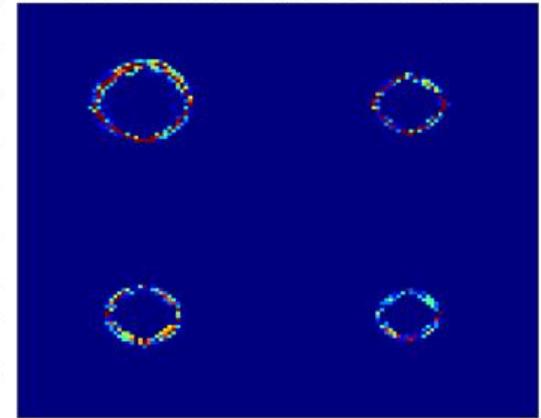
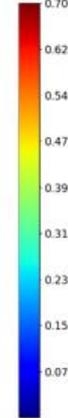
CMG (L: 09 of Blind_Run_5.0)



2023-01-01 (L: 09 of Blind_Run_5.0)



2023-01-01 Percent Error(L: 09 of Blind_Run_5.0)



CMG - Numerical Reservoir Simulation

Smart Proxy Model

%Error

January 2023



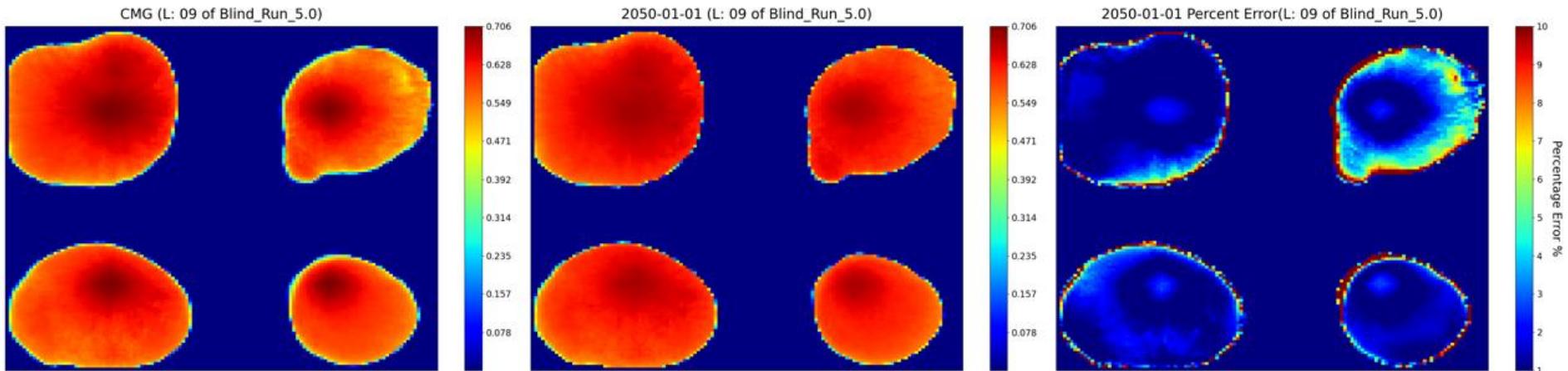
**Annual Distribution
CO₂ Saturation**

**From: January 2023
To: January 2050**

Blind Validation

Geological Realization #5, Layer 9

CO₂ Saturation Distribution Video



CMG - Numerical Reservoir Simulation

Smart Proxy Model

%Error

January 2050



**Annual Distribution
CO₂ Saturation**

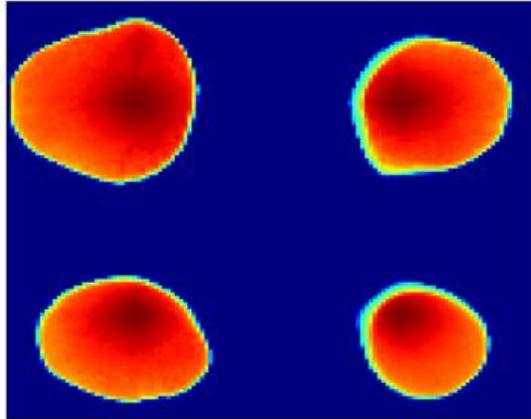
**From: January 2023
To: January 2050**

Blind Validation

Geological Realization #5, Layer 9

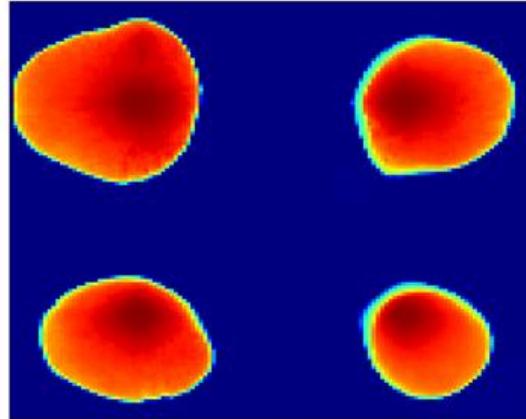
CO₂ Saturation Distribution Video

CMG (L: 14 of Blind_Run_5.0)



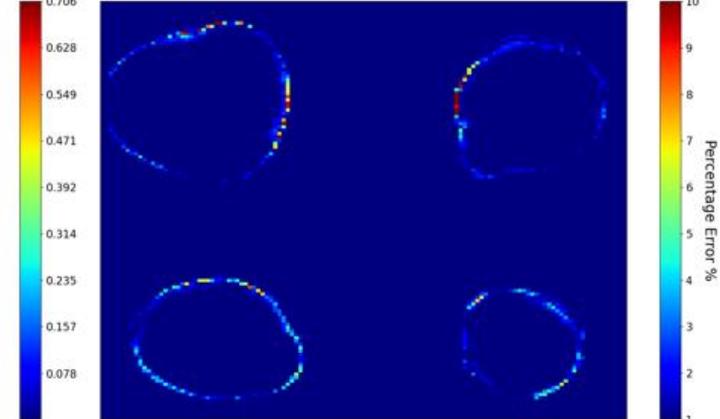
CMG - Numerical Reservoir Simulation

2051-01-01 (L: 14 of Blind_Run_5.0)



Smart Proxy Model

2051-01-01 Percent Error(L: 14 of Blind_Run_5.0)



%Error

January 2051



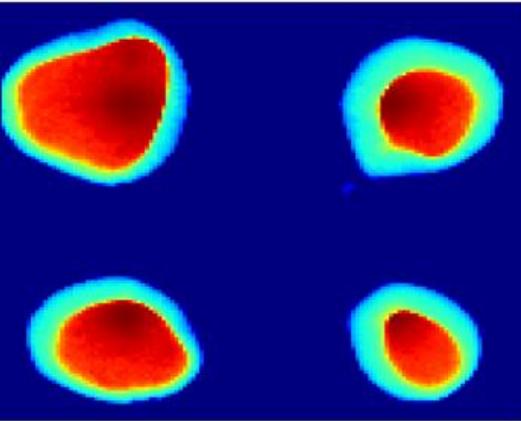
**Annual Distribution
CO₂ Saturation**

From: January 2051
To: January 2070

**Blind Validation
Geological Realization #5, Layer I4**

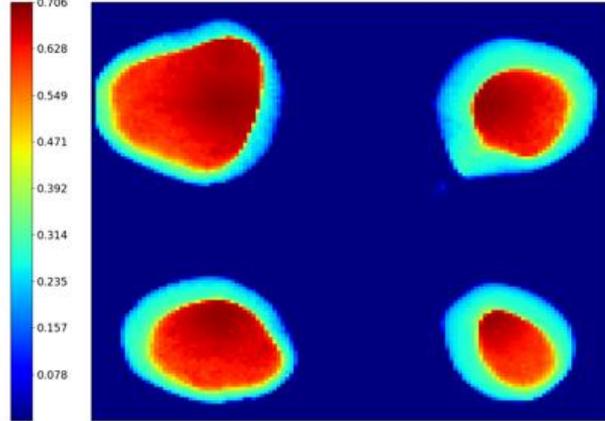
CO₂ Saturation Distribution Video

CMG (L: 14 of Blind_Run_5.0)



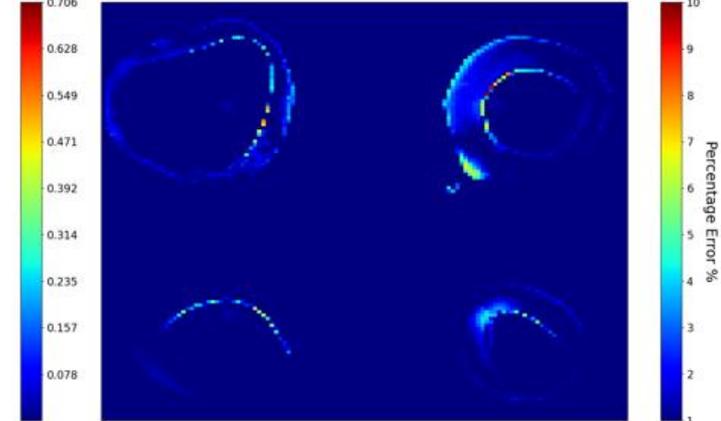
CMG - Numerical Reservoir Simulation

2070-01-01 (L: 14 of Blind_Run_5.0)



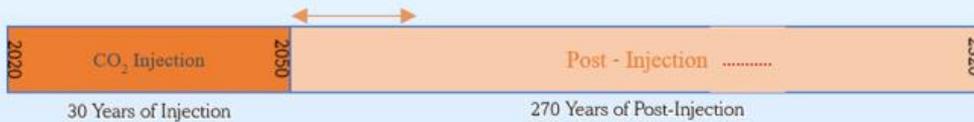
Smart Proxy Model

2070-01-01 Percent Error(L: 14 of Blind_Run_5.0)



%Error

January 2070



Annual Distribution
CO₂ Saturation

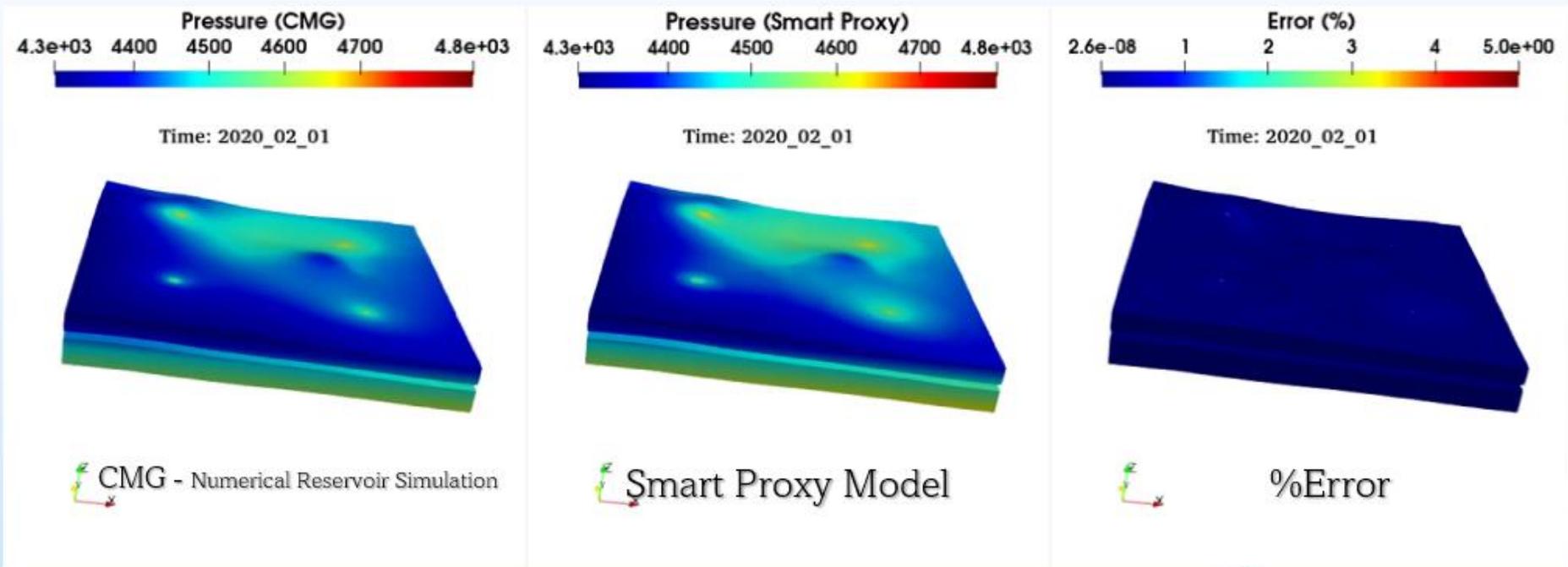
From: January 2051
To: January 2070

Blind Validation

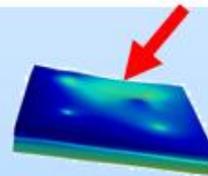
Geological Realization #5, Layer 14

BLIND RUN #5 – 3-D in Space & Time

Dynamic Reservoir Pressure

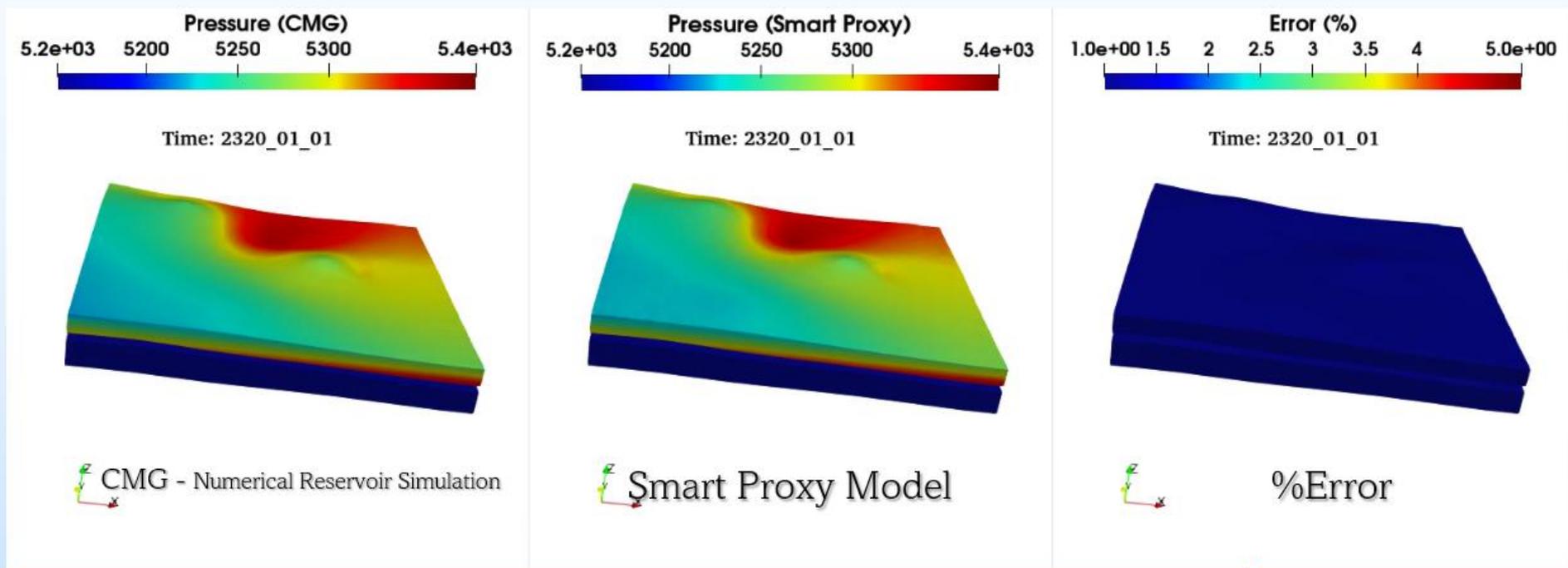


Looking from the **Top**

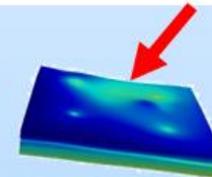


BLIND RUN #5 – 3-D in Space & Time

Dynamic Reservoir Pressure

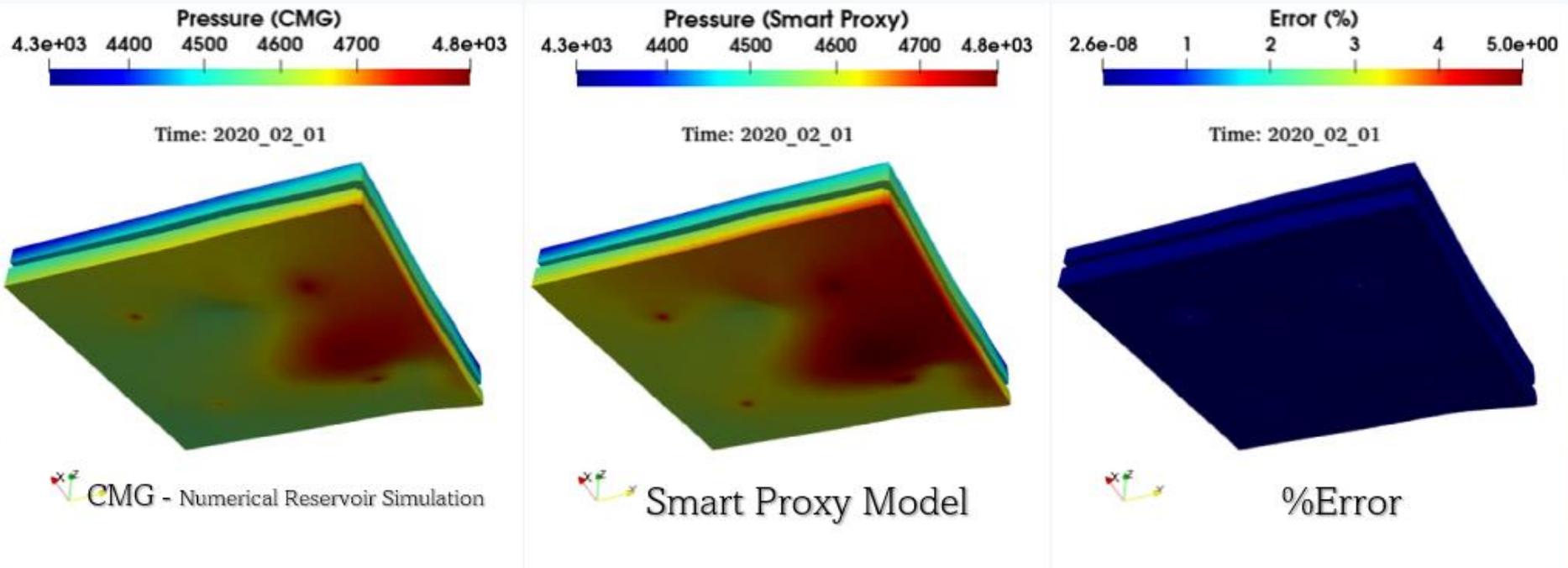


Looking from the **Top**

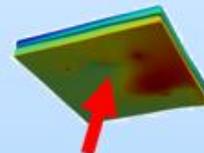


BLIND RUN #5 – 3-D in Space & Time

Dynamic Reservoir Pressure

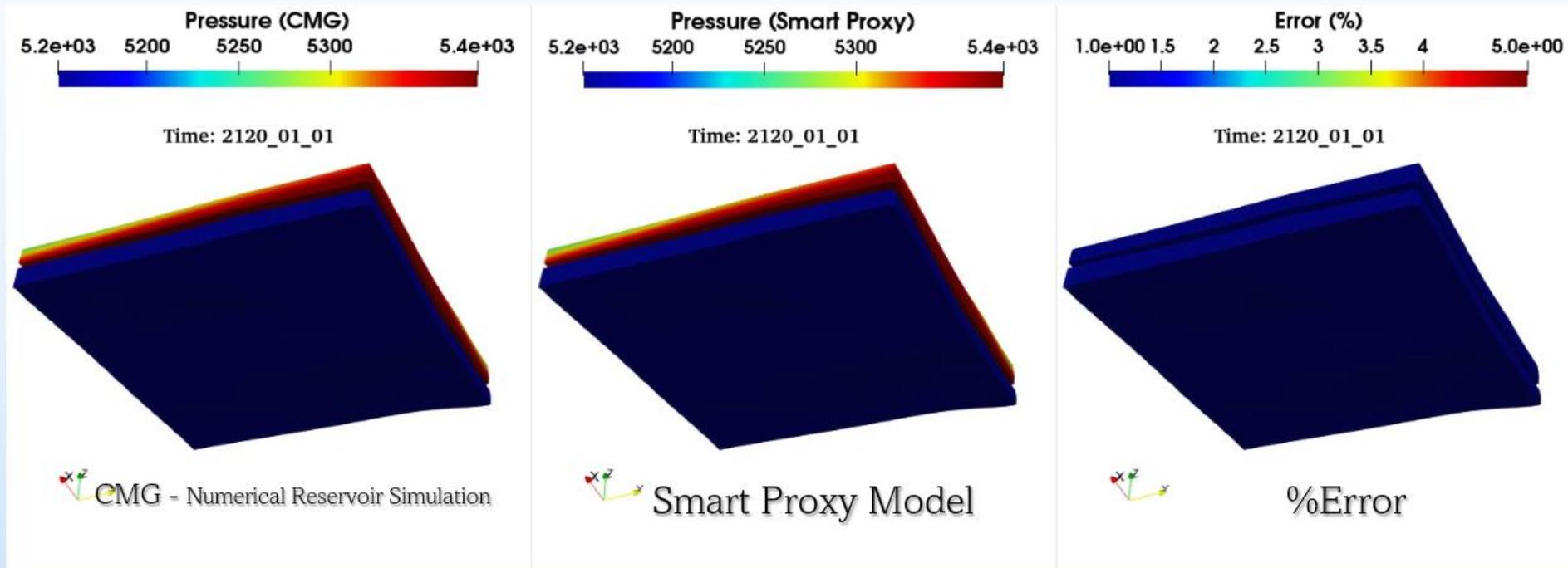


Looking from the **Bottom**

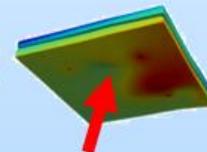


BLIND RUN #5 – 3-D in Space & Time

Dynamic Reservoir Pressure

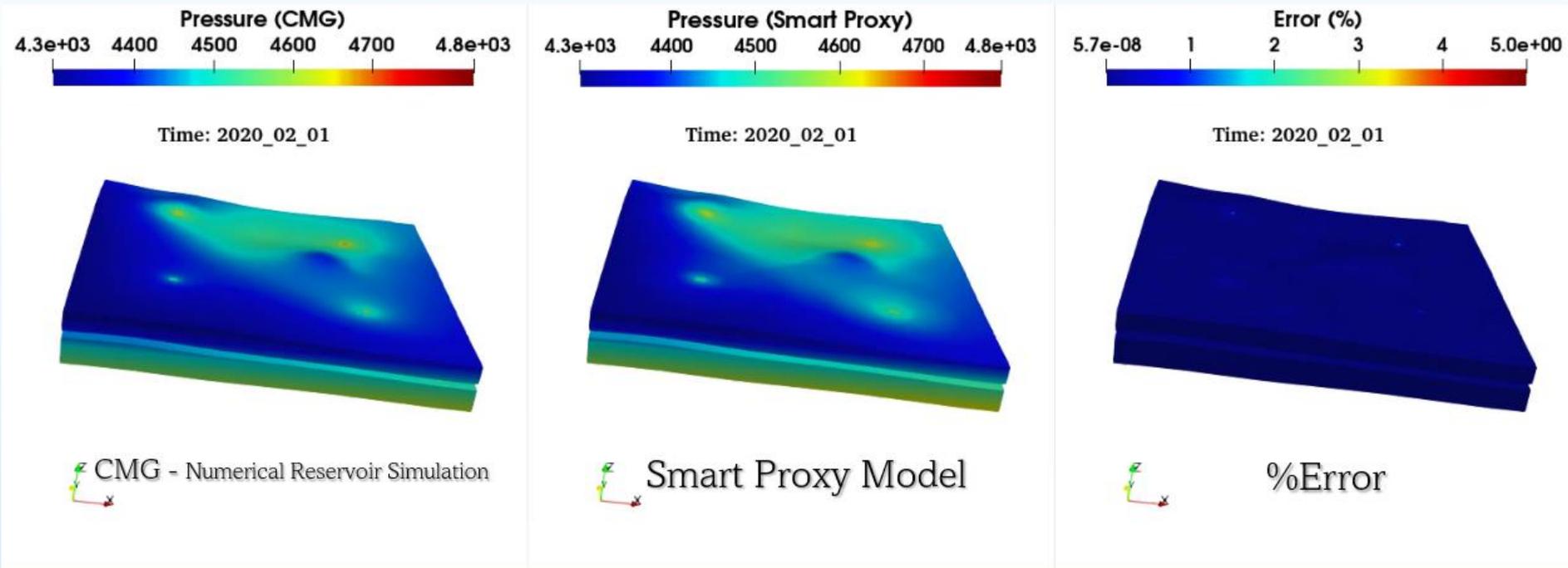


Looking from the **Bottom**

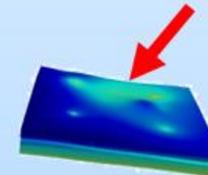


BLIND RUN #13 – 3-D in Space & Time

Dynamic Reservoir Pressure



Looking from the **Top**

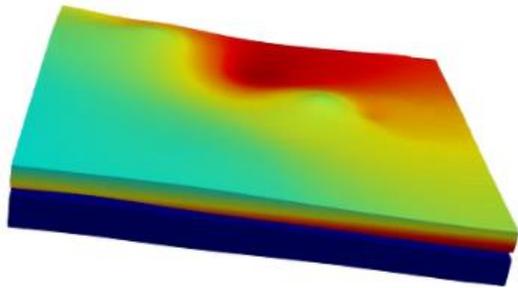


BLIND RUN #13 – 3-D in Space & Time

Dynamic Reservoir Pressure

Pressure (CMG)
5.2e+03 5200 5250 5300 5.4e+03

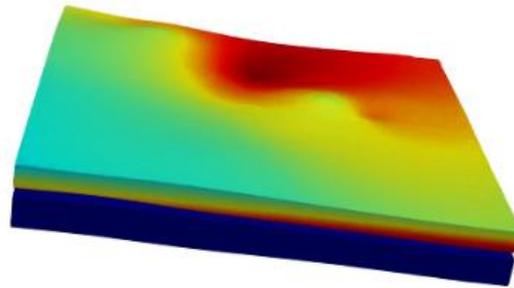
Time: 2120_01_01



CMG - Numerical Reservoir Simulation

Pressure (Smart Proxy)
5.2e+03 5200 5250 5300 5.4e+03

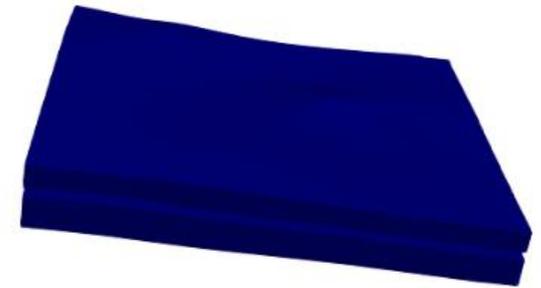
Time: 2120_01_01



Smart Proxy Model

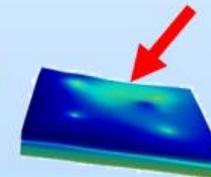
Error (%)
1.0e+00 1.5 2 2.5 3 3.5 4 5.0e+00

Time: 2120_01_01



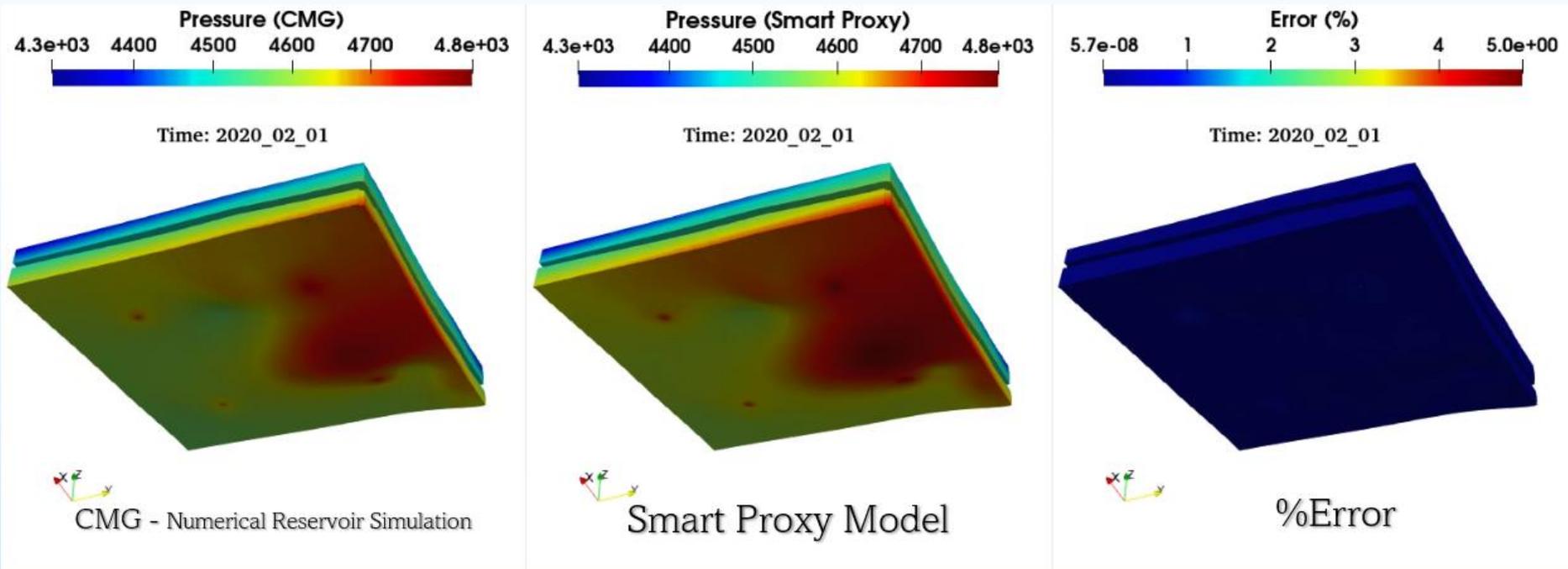
%Error

Looking from the **Top**

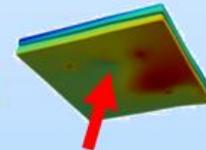


BLIND RUN #13 – 3-D in Space & Time

Dynamic Reservoir Pressure

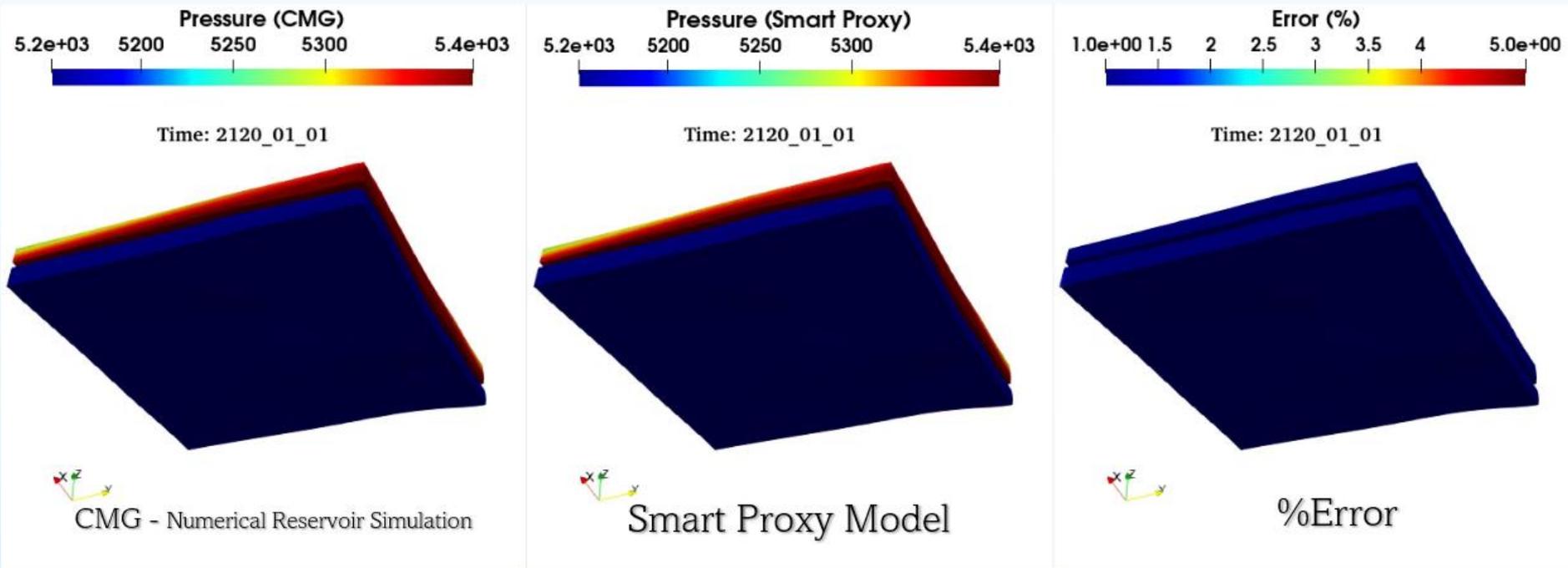


Looking from the **Bottom**

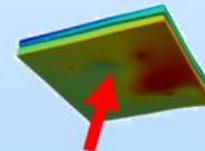


BLIND RUN #13 – 3-D in Space & Time

Dynamic Reservoir Pressure



Looking from the **Bottom**

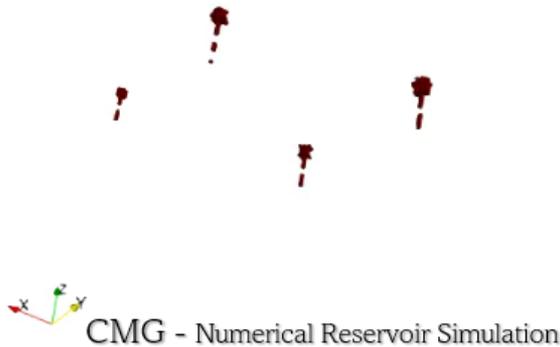


BLIND RUN #5 – 3-D in Space & Time

Dynamic CO₂ Saturation

CMG CO2 Plume (Sat. > 10%)

Time: 2020_02_01



Smart Proxy CO2 Plume (Sat. > 10%)

Time: 2020_02_01

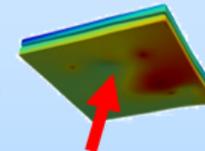


Prediction Accuracy

Time: 2020_02_01



Looking from the **Bottom**



BLIND RUN #5 – 3-D in Space & Time

Dynamic CO₂ Saturation

CMG CO2 Plume (Sat. > 10%)

Time: 2170_01_01



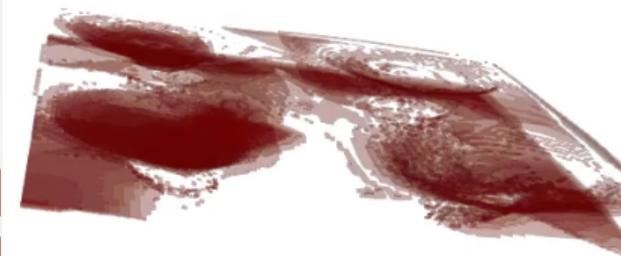
Smart Proxy CO2 Plume (Sat. > 10%)

Time: 2170_01_01



Prediction Accuracy

Time: 2170_01_01

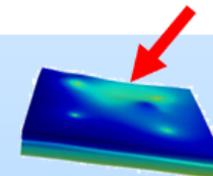


 CMG - Numerical Reservoir Simulation

 Smart Proxy Model

 %Error

Looking from the Top

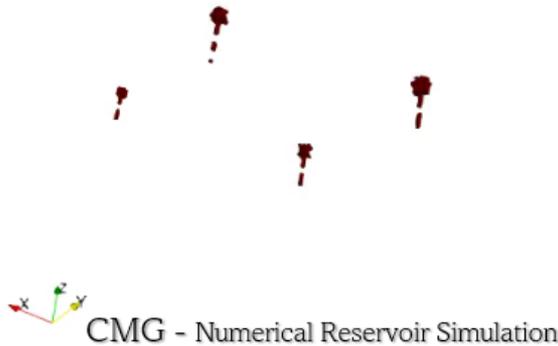


BLIND RUN #5 – 3-D in Space & Time

Dynamic CO₂ Saturation

CMG CO2 Plume (Sat. > 10%)

Time: 2020_02_01



Smart Proxy CO2 Plume (Sat. > 10%)

Time: 2020_02_01

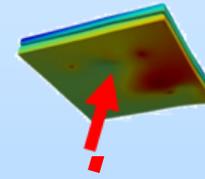


Prediction Accuracy

Time: 2020_02_01



Looking from the **Bottom**



BLIND RUN #5 – 3-D in Space & Time

Dynamic CO₂ Saturation

CMG CO2 Plume (Sat. > 10%)

Time: 2320_01_01



 CMG - Numerical Reservoir Simulation

Smart Proxy CO2 Plume (Sat. > 10%)

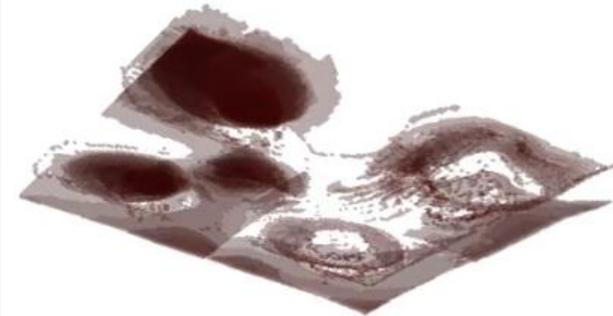
Time: 2320_01_01



 Smart Proxy Model

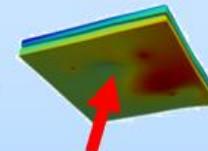
Prediction Accuracy

Time: 2320_01_01



 %Error

Looking from the **Bottom**

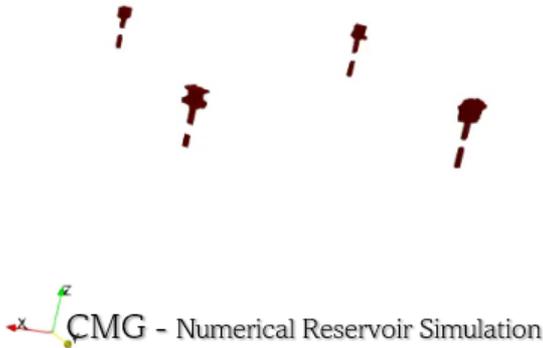


BLIND RUN #13 – 3-D in Space & Time

Dynamic CO₂ Saturation

CMG CO2 Plume (Sat. > 10%)

Time: 2020_02_01



Smart Proxy CO2 Plume (Sat. > 10%)

Time: 2020_02_01

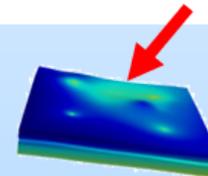


Prediction Accuracy

Time: 2020_02_01



Looking from the **Top**

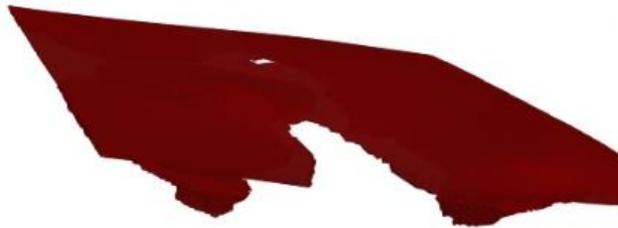


BLIND RUN #13 – 3-D in Space & Time

Dynamic CO₂ Saturation

CMG CO₂ Plume (Sat. > 10%)

Time: 2320_01_01



 CMG - Numerical Reservoir Simulation

Smart Proxy CO₂ Plume (Sat. > 10%)

Time: 2320_01_01



 Smart Proxy Model

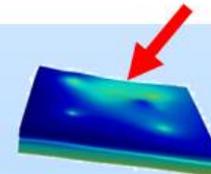
Prediction Accuracy

Time: 2320_01_01



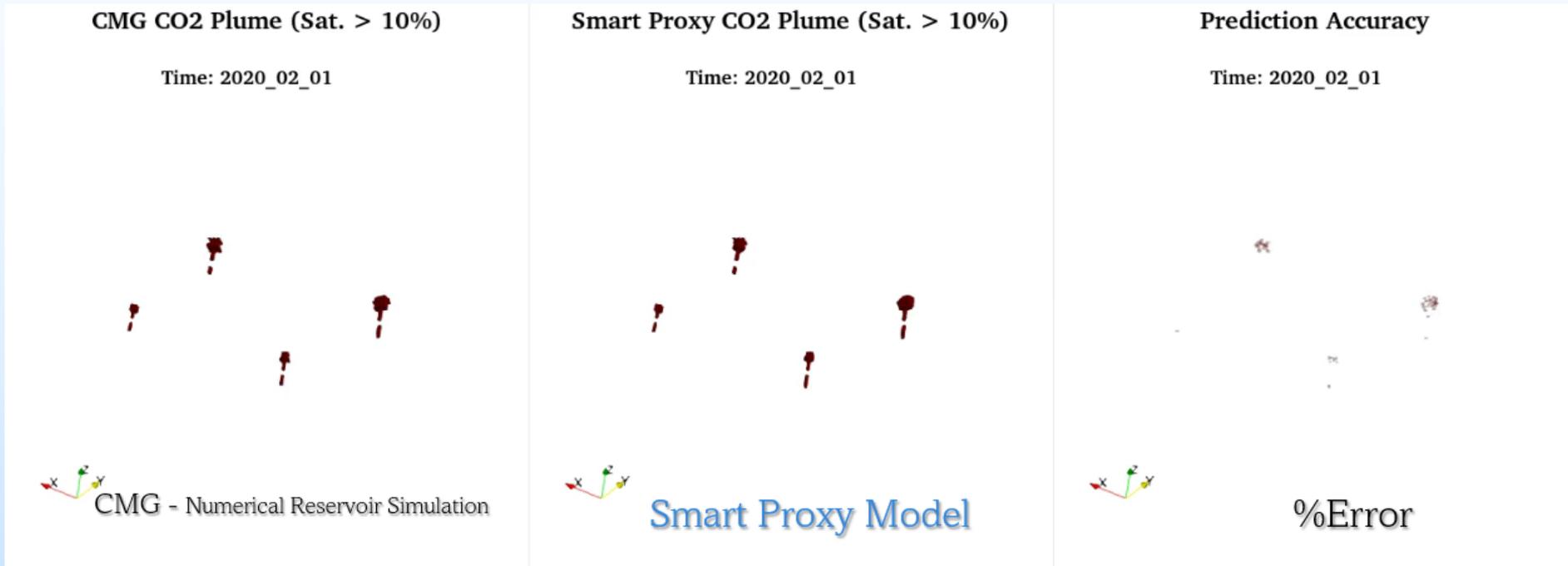
 %Error

Looking from the **Top**

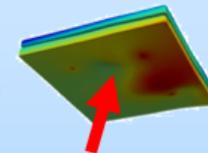


BLIND RUN #13 – 3-D in Space & Time

Dynamic CO₂ Saturation



Looking from the **Bottom**



BLIND RUN #13 – 3-D in Space & Time

Dynamic CO₂ Saturation

CMG CO2 Plume (Sat. > 10%)

Time: 2170_01_01



 CMG - Numerical Reservoir Simulation

Smart Proxy CO2 Plume (Sat. > 10%)

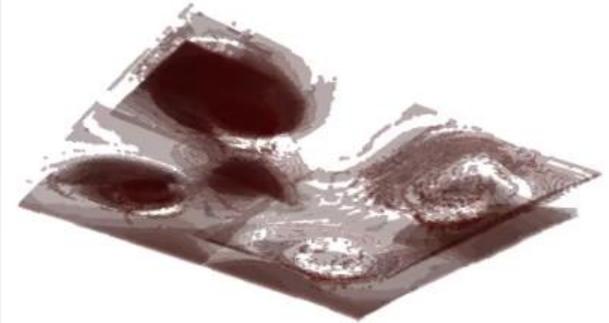
Time: 2170_01_01



 Smart Proxy Model

Prediction Accuracy

Time: 2170_01_01



 %Error

Looking from the **Bottom**

