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Deep Learning Emulators for Pore-Scale CO2-Water Interaction

CHI4Science Group

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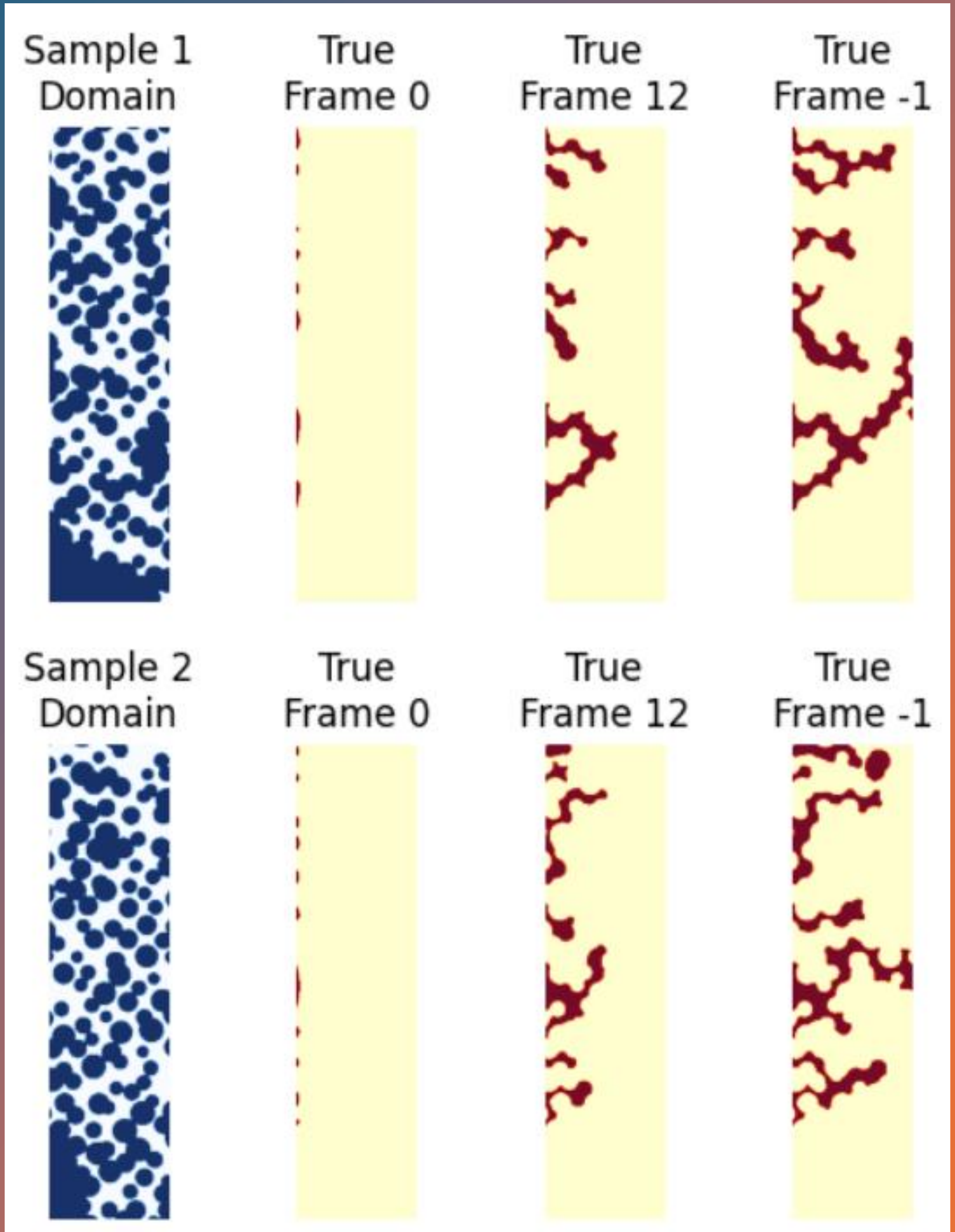

Hackathon Challenge : CO2-Water Interaction Emulator at the Pore-Scale

- **Goal:** Develop a fast, accurate emulator to predict CO_2 invasion in porous media
- **Dataset:** Binary domain images (512 × 128) and CO_2 invasion time series (25 time steps)
- **Challenge:** Predict CO_2 displacement from initial geometry while ensuring physical consistency and generalization to new domains
- **Key Factors:** Complex flow dynamics, physical constraints (constant flow rate up to **breakthrough**), **capillary-driven retraction or backflow**, uncertainties, speed & efficiency

(Really!) Recent developments on hybrid approaches

FluidNet-Lite: Lightweight Convolutional Neural Network for Pore-scale Modeling of Multiphase Flow in Heterogeneous Porous Media

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ARTICLE INFO

Keywords:
Multiphase flow
viscosity ratio
contact angle
fluid displacement dynamics
computational efficiency
surrogate models
physics-informed CNNs
real-time fluid simulation

ABSTRACT

Modeling breakthrough patterns in heterogeneous porous media during two-phase fluid flow presents unique challenges due to computational complexity and data scarcity. Current deep learning approaches, primarily generative adversarial network (GAN) based, focus on homogeneous media, limiting their practical application in real-world heterogeneous pore systems. In this work, we introduce *FluidNet-Lite*, a lightweight Convolutional Neural Network for pore-scale modeling in heterogeneous porous media. Departing from generative task frameworks, we reformulate breakthrough pattern prediction as an innovative pixel-wise classification task, significantly reducing model complexity. By integrating two essential physical parameters—viscosity ratio (M) and contact angle (θ), our approach improves predictive accuracy and embeds critical physics-based dependencies directly into the learning process. A Grain-Weighted Adaptive Loss (GWAL) function further enforces fluid flow principles, enhancing model consistency with physical laws. *FluidNet-Lite* achieves state-of-the-art performance with an Intersection over Union (IoU) of 0.92 and a Structural Similarity Index Measure (SSIM) of 0.89. It is 94% lighter and 48% more computationally efficient than GAN-based alternatives, reducing VRAM usage by 40% and inference time by 30%. Demonstrating robust generalization across interpolation, extrapolation, and unseen test samples, *FluidNet-Lite* sets a new benchmark for lightweight, physics-informed modeling in heterogeneous porous media fluid dynamics, as evidenced by its superior performance and efficiency improvements over conventional approaches. We also publish a comprehensive dataset and codebase to support future research in lightweight architectures for deep learning-based surrogate modeling of pore-scale immiscible displacement patterns.

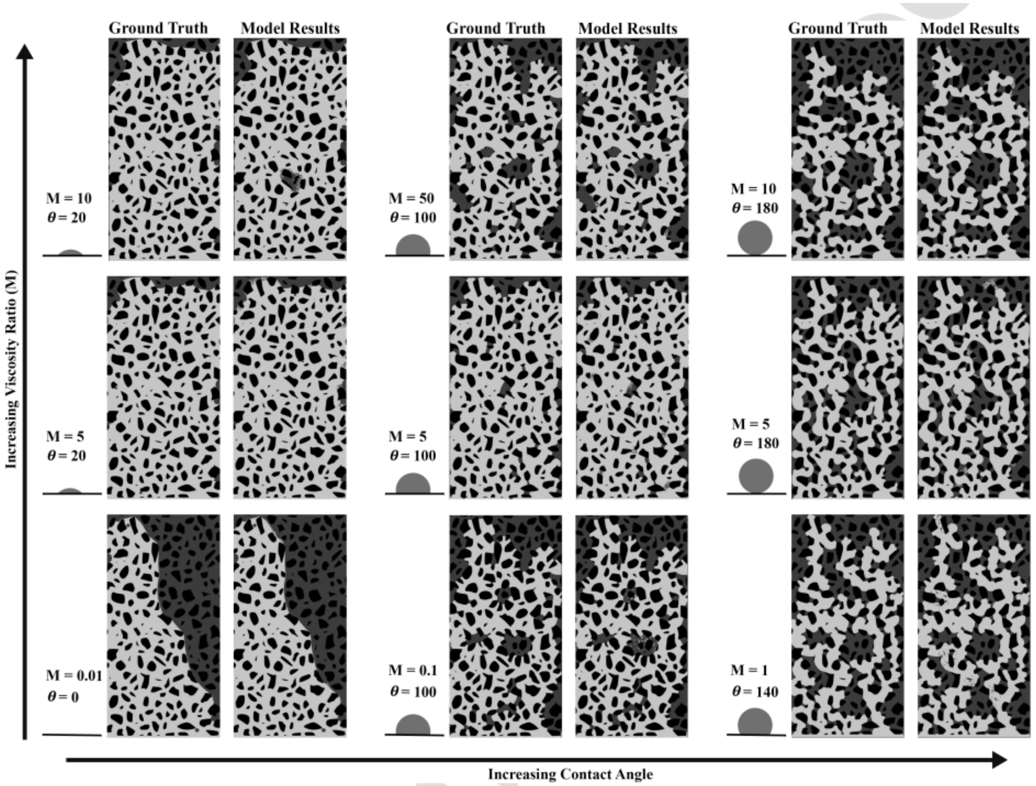


Figure 5: *Model Performance under different scenarios* Model results showing the ground truth and the model prediction for different scenarios and the same pore geometry.

First approach: Predict specific time steps (dynamic residual predictions)

- **Idea:** Predict residual (differential) changes between time steps instead of state at a given time

- **Why ?**

Try to **capture backflow** due to pressure effects

Account for global contributions of invasion and backflow patterns at given time step

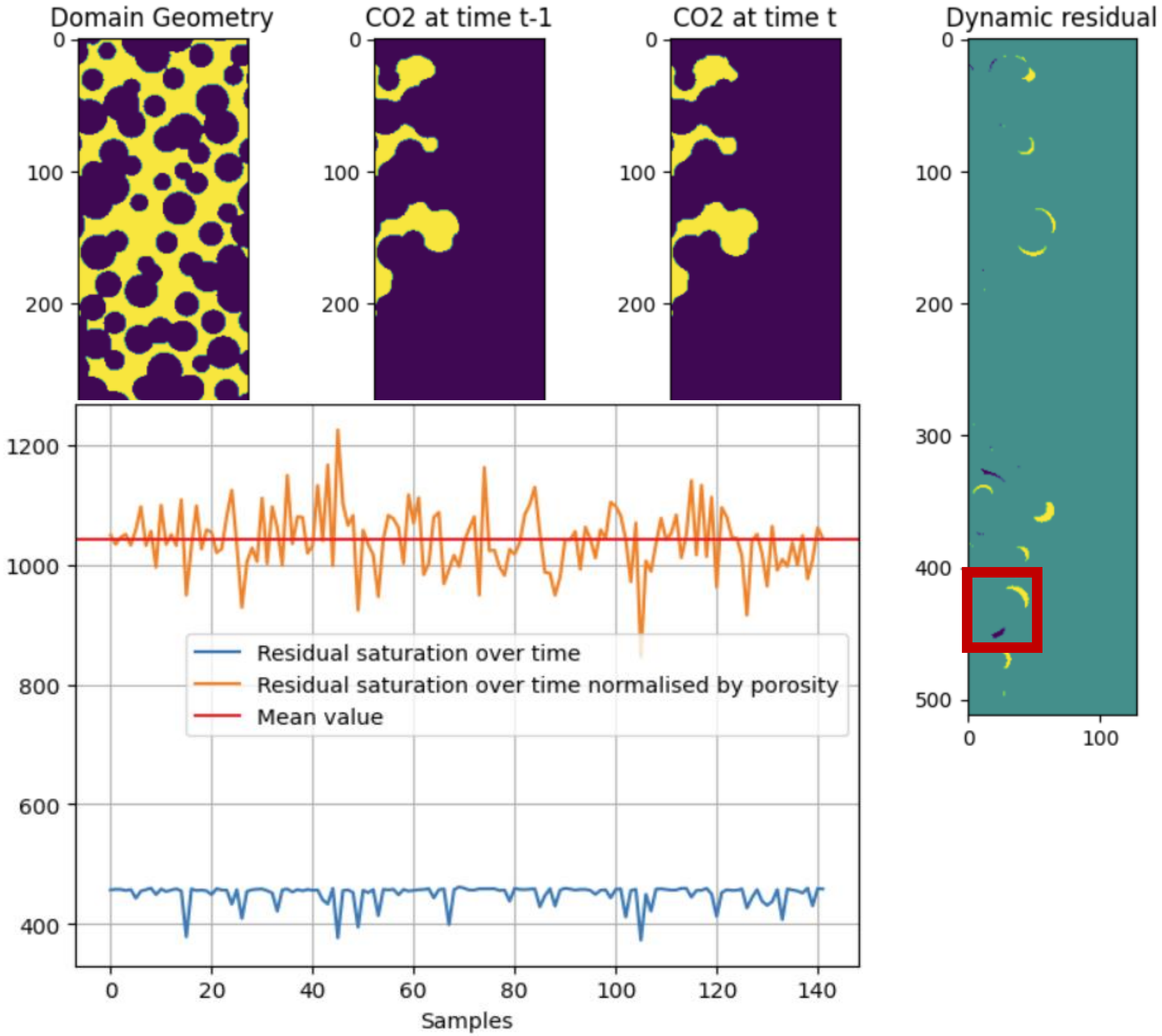
Impose physics – Constant flow rate over time across all samples – *Mass conservation*

- **Challenges**

Multi-class classification (3 classes) with **highly imbalanced classes - Weighted CE loss / Focal loss**

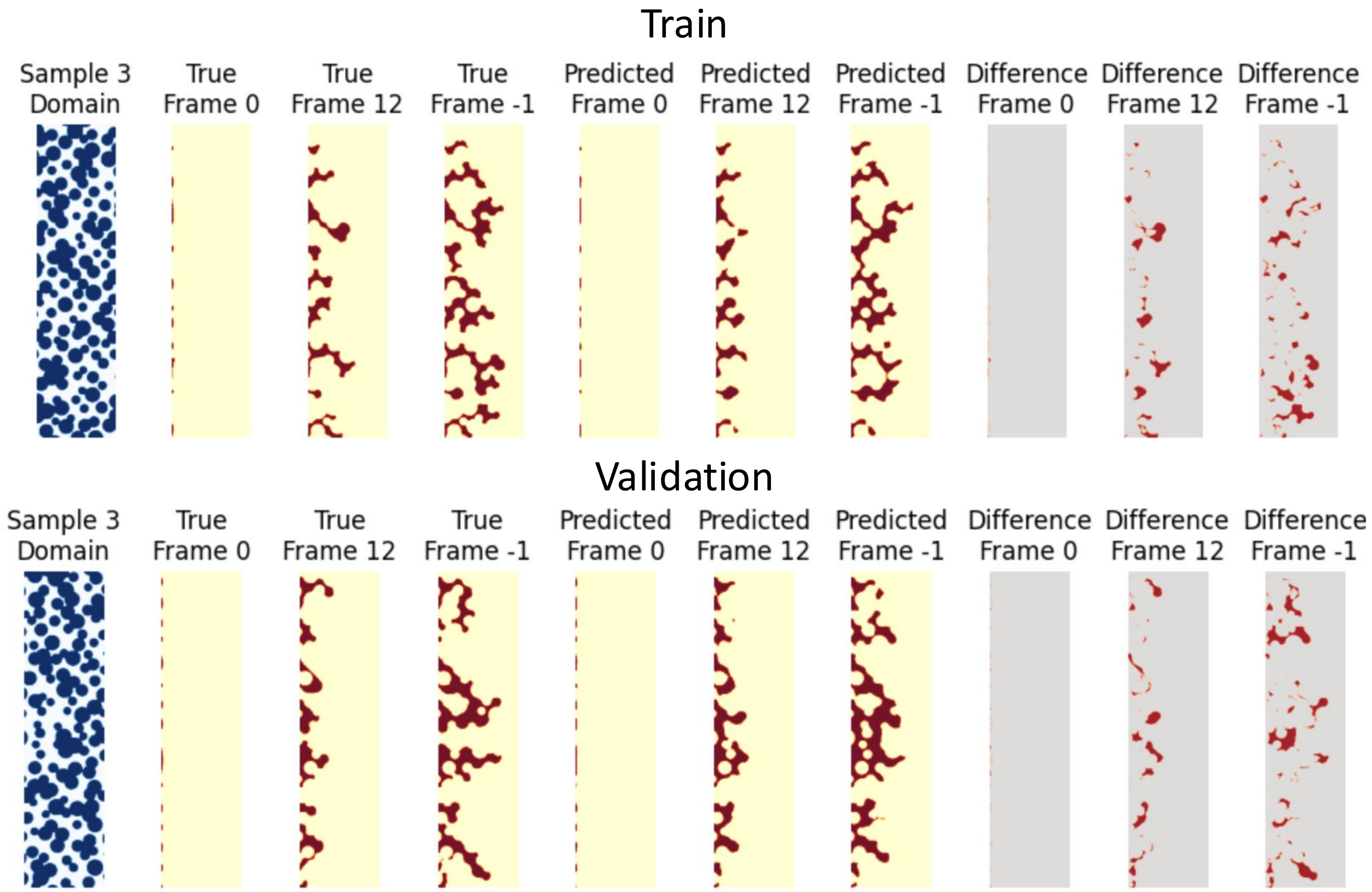
Disconnected geometries, difficult to capture

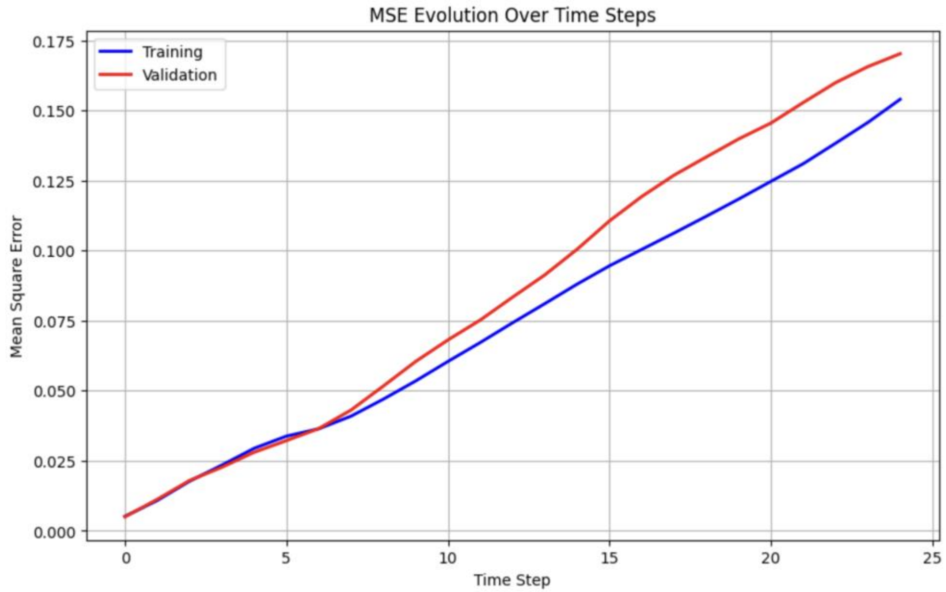
Uncertainties - **Stochastic perturbation of physics loss** - Mass conservation on validation samples may not be guaranteed !



Second approach: Predict specific time steps (state predictions)

- **Idea:** U-ResNet with Spatial Attention mechanism, Dice Loss & Focal Loss
- **Challenges:** Worse Performance in unseen data





Average Train MSE: 0.075786 vs. 0.092671 (orig.)

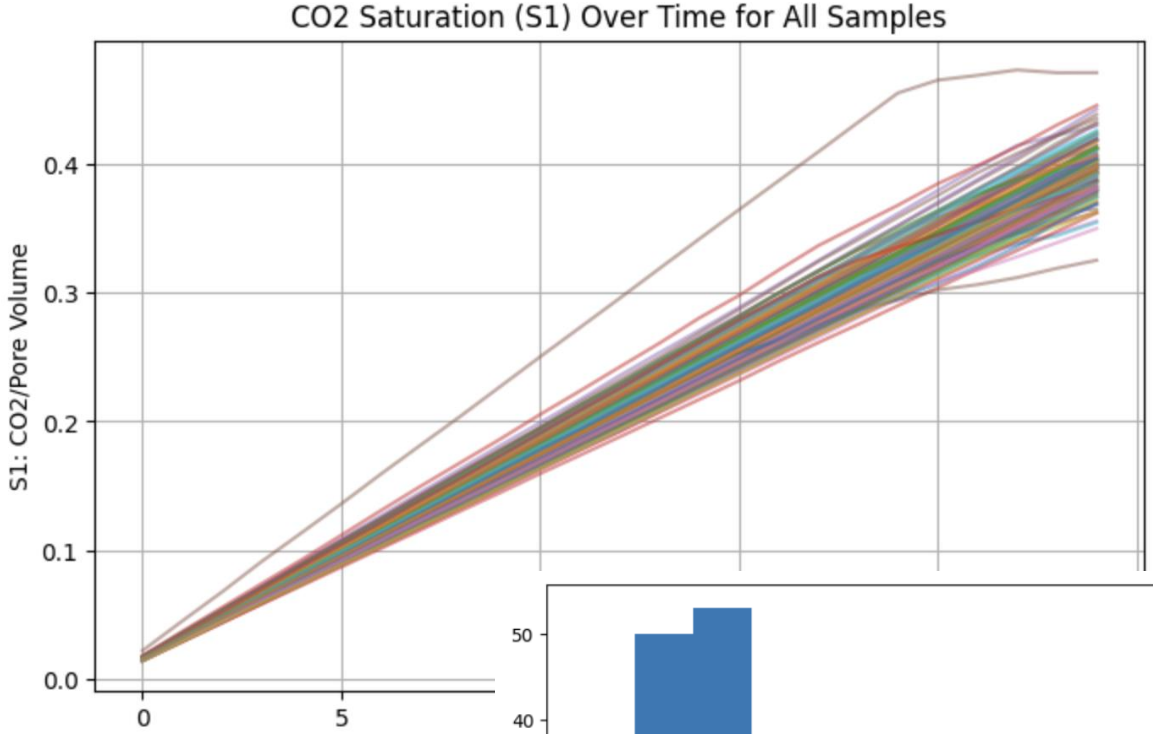
Average Val MSE: 0.086053 vs. 0.093952

Final Time Step Train MSE: 0.153957 vs. 0.189575

Final Time Step Val MSE: 0.170212 vs. 0.190245

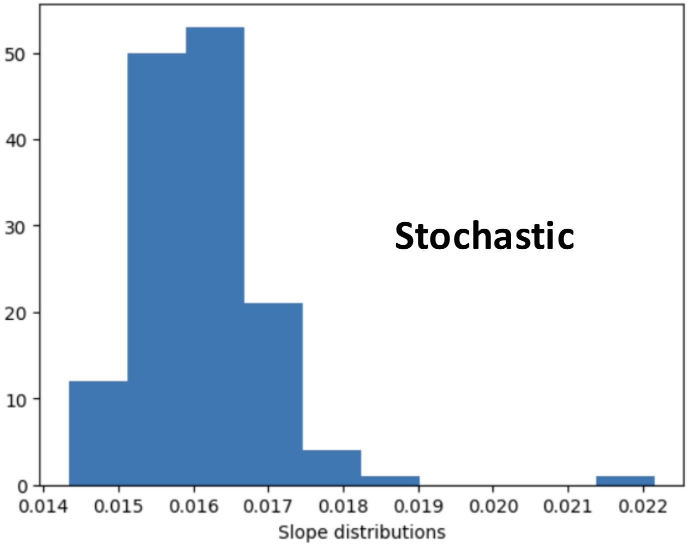
Second approach: Predict specific time steps (state predictions)

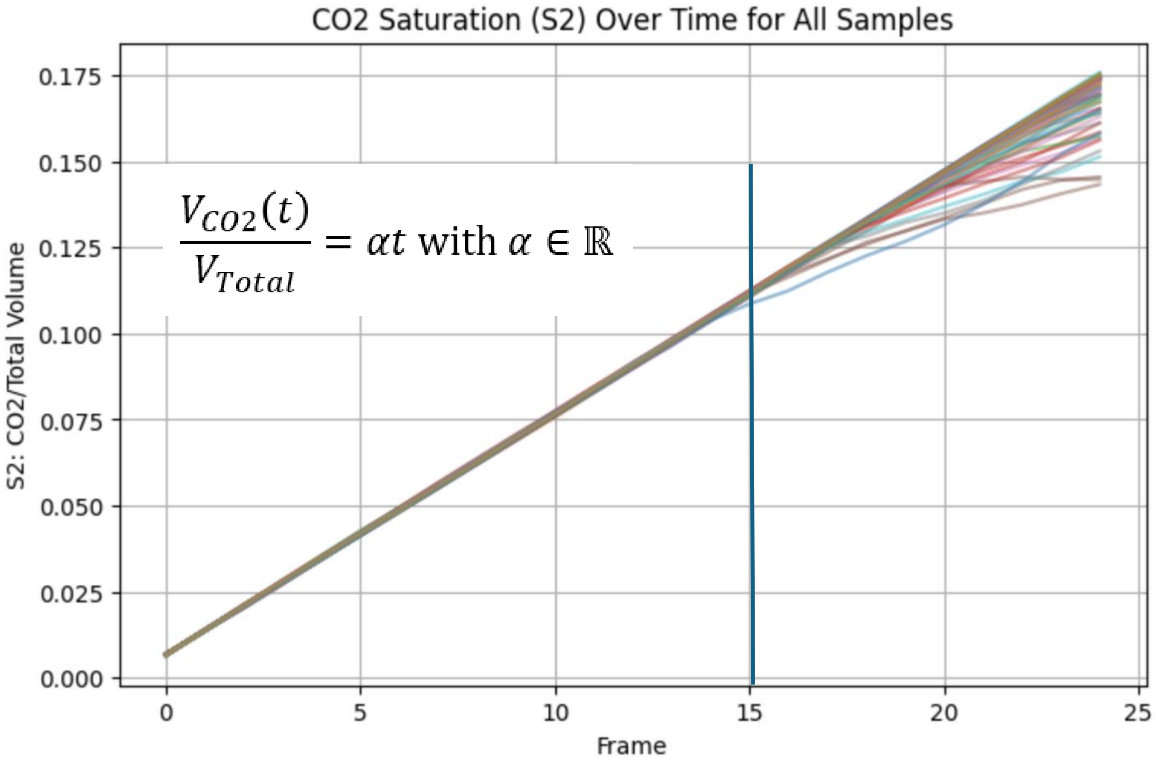
- **Idea:** U-ResNet with Spatial Attention mechanism, Dice Loss & Focal Loss, and Physics_Loss (**stochastic**)



$$\frac{V_{CO2}(t)}{V_{pores}} = \xi t$$

$$with \quad \xi \sim \mathcal{N}(s_{mean}, \sigma^2)$$



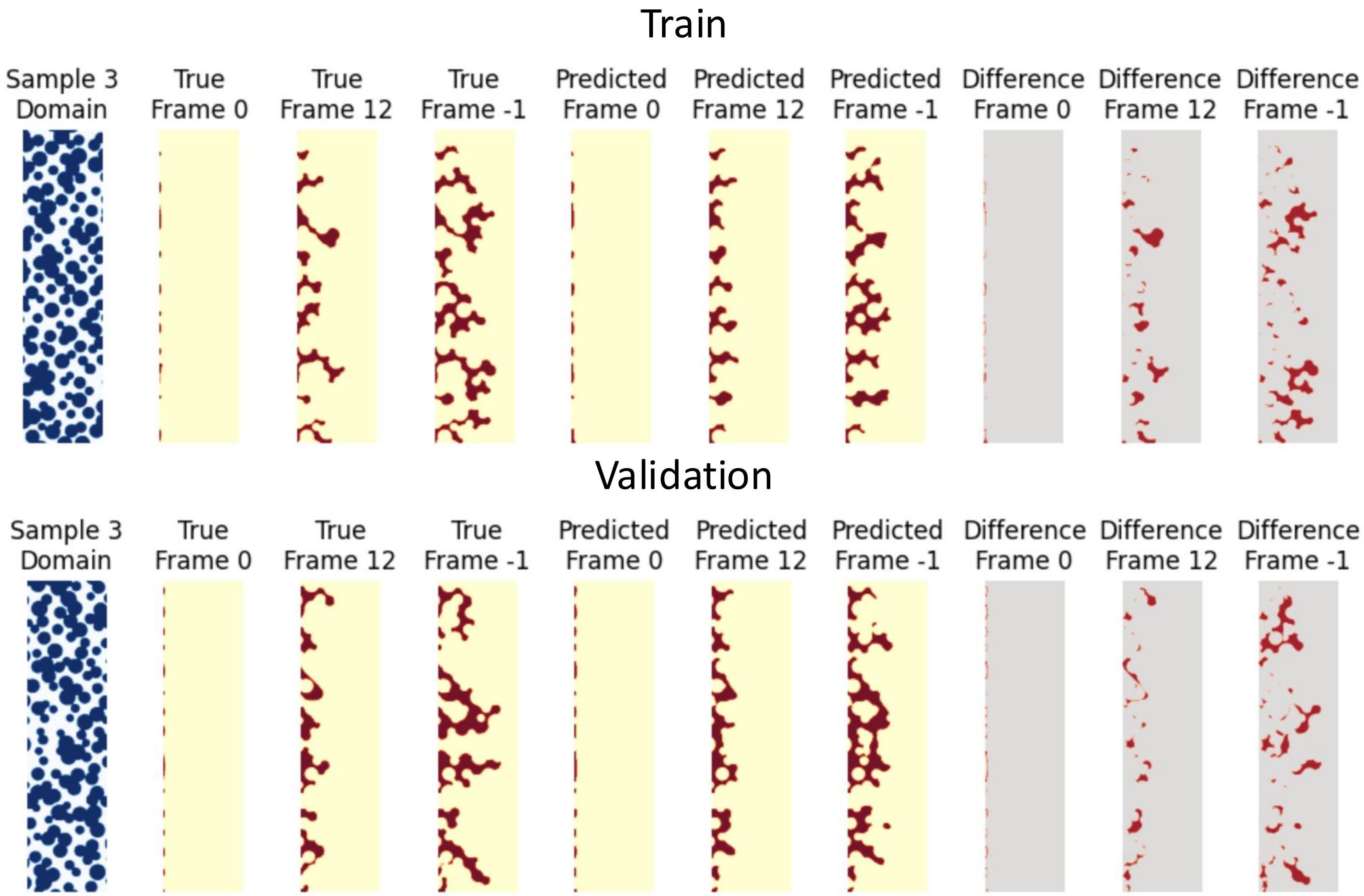


$$\frac{V_{CO2}(t)}{V_{Total}} = \alpha t \text{ with } \alpha \in \mathbb{R}$$

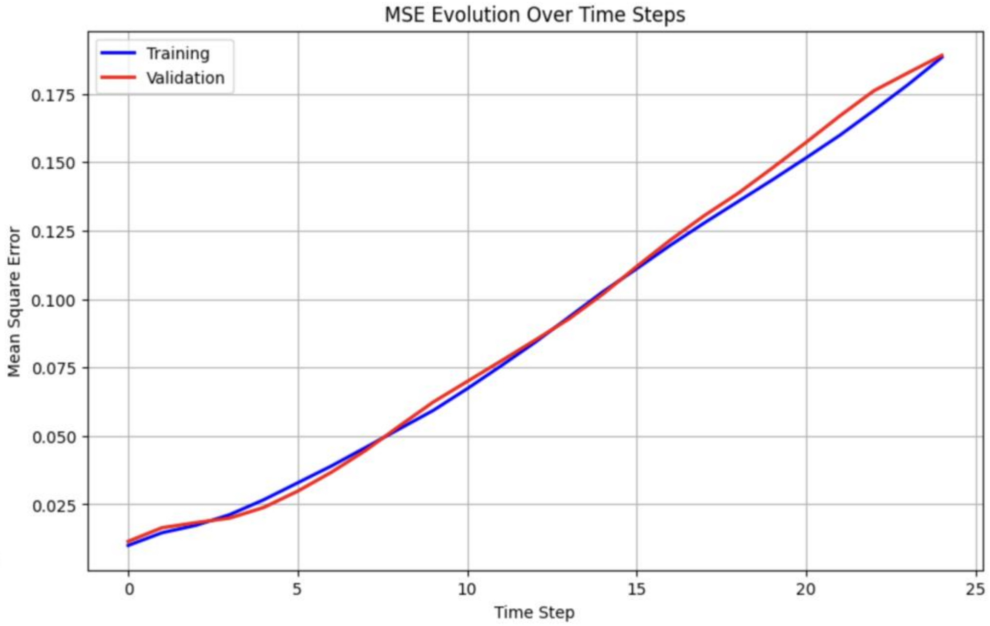
Deterministic until time step 15

Second approach: Predict specific time steps (state predictions)

- **Idea:** U-ResNet with Spatial Attention mechanism, Dice Loss & Focal Loss, and Physics_Loss (**stochastic**)
- **Challenge:** Improved performance on unseen data, but overall ability wasn't improved



Dice Loss and Physics_Loss (**stochastic**)



Average Train MSE: 0.089110 vs. 0.092671 (orig.)

Average Val MSE: 0.090683 vs. 0.093952

Final Time Step Train MSE: 0.188382 vs. 0.189575

Final Time Step Val MSE: 0.189101 vs. 0.190245

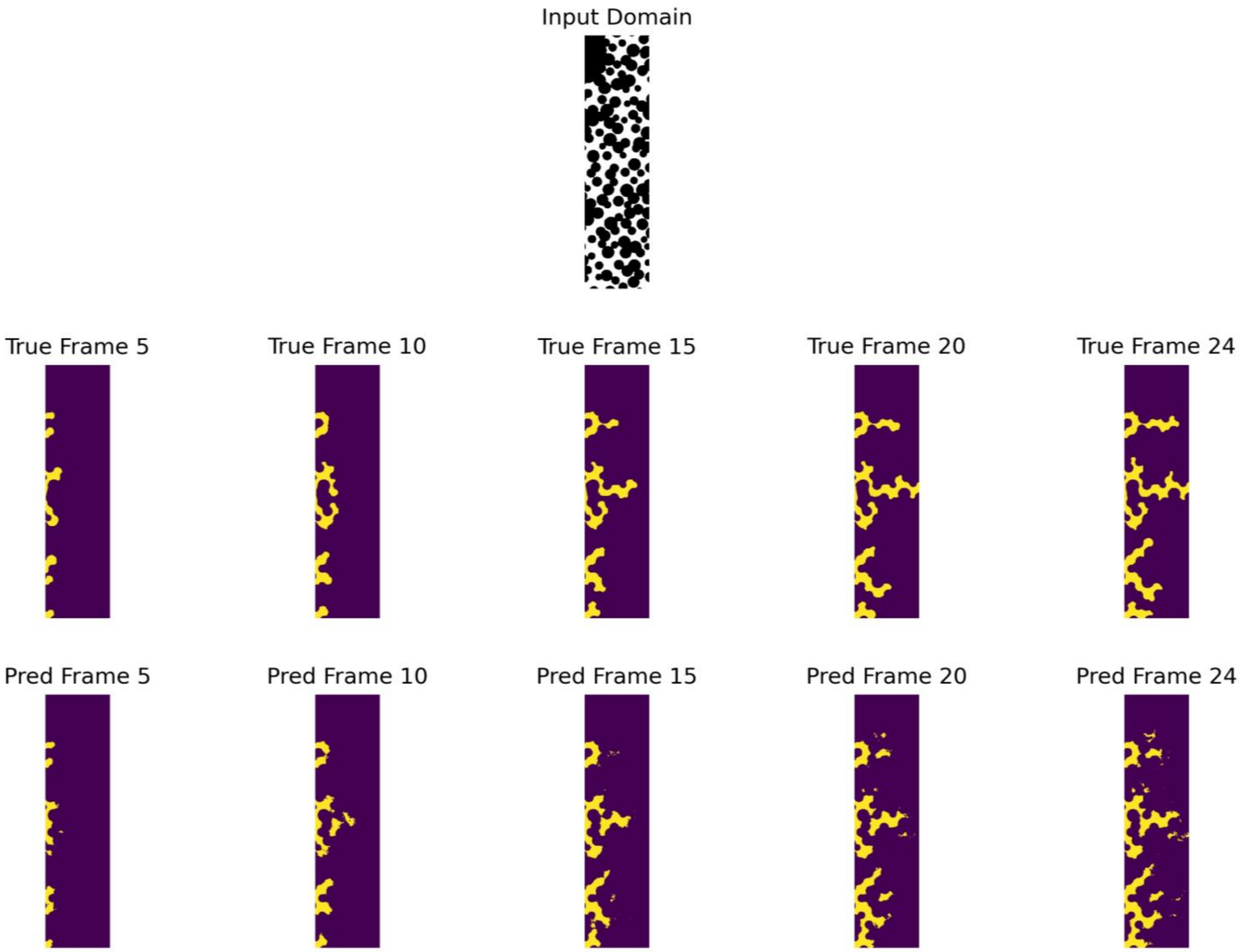
Third approach: Predict all 25 time frames together

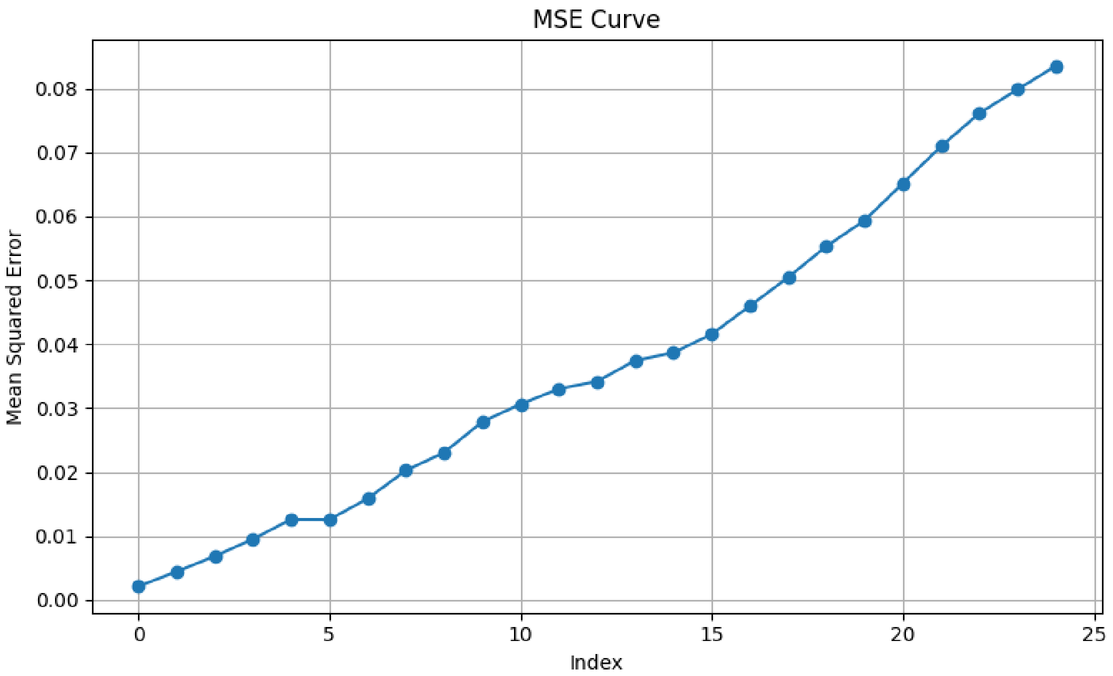
Model Name	Diffusion?	Attention?	Physics Loss?	FocalLoss	MSE Loss	BCELoss	Model metric\AVE RAGE Mean square error
UNetAttnPhysics	✗	✓	✓	✗	✗	✓	0.0390
UNetAttnCE	✗	✓	✗	✗	✗	✓	0.0386
UNetAttnMSE	✗	✓	✗	✗	✓	✗	0.0396
UNetAttnFocal	✗	✗	✗	✓	✗	✗	0.0394
UNETMSE	✗	✗	✗	✗	✓	✗	0.0399
DiffUnetAtten	✓	✗	✗	✗	✓	✗	0.0453

Time comsuming and Memory Cost: (inference batchsize=10 and inference on 512x512)
Model with 1 output channel - Time: 1.35 /10/1s, Max memory: 3729.39 MB
Model with 25 output channels - Time: 1.55/10/25 s, Max memory: 3777.39 MB
Model with 100 output channels - Time: 1.56/10/25 s, Max memory: 3927.39 MB

Model Plan and Model result

Model result Analysis





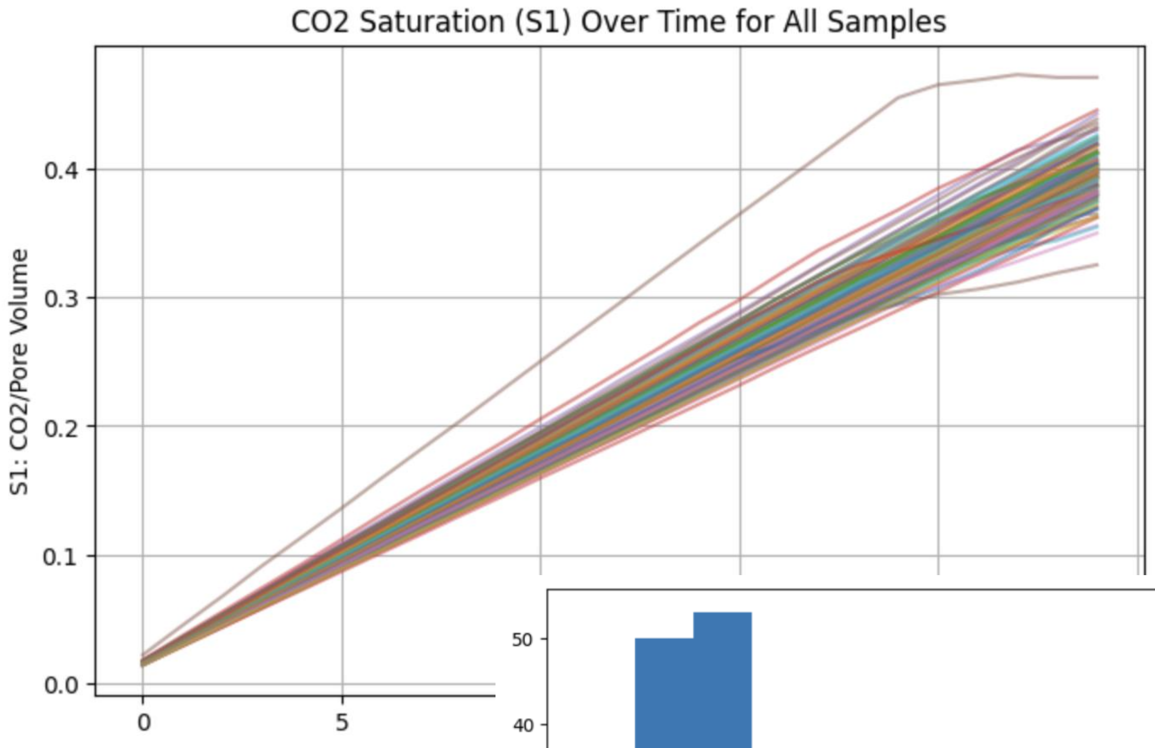
Average Val MSE: 0.0386 vs. 0.0940

The later timestep, the bigger the loss.

Later result is hard to learn.

Physics might within the data pattern.

Open Questions & Discussion



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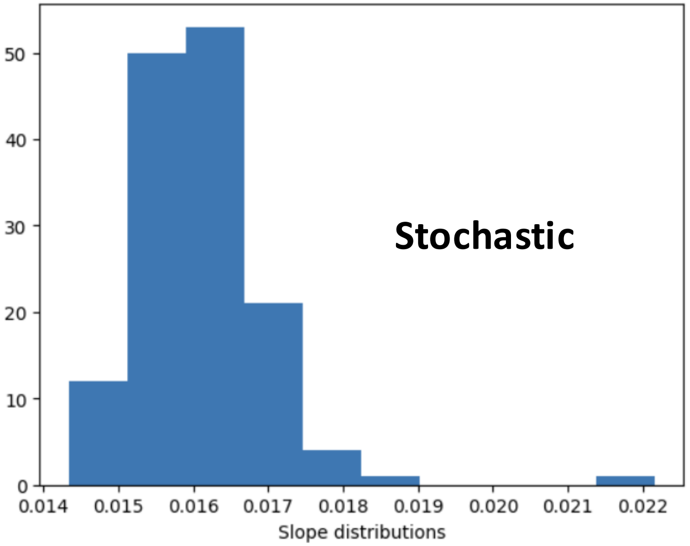
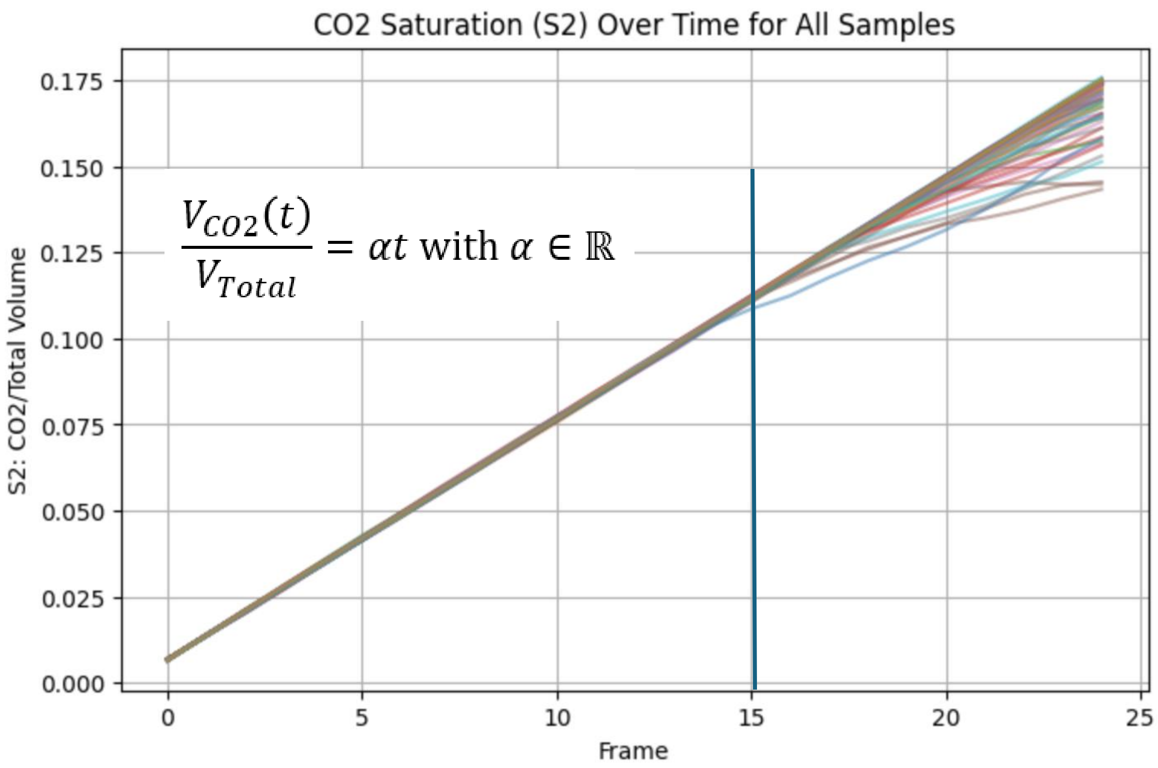


Stochastic



$$\frac{V_{CO2}(t)}{V_{Total}} = \alpha t \text{ with } \alpha \in \mathbb{R}$$

Deterministic until time step 15

Thank you !