Data-driven Models of Adsorption Equilibria of Multi-component Mixtures in Porous Materials

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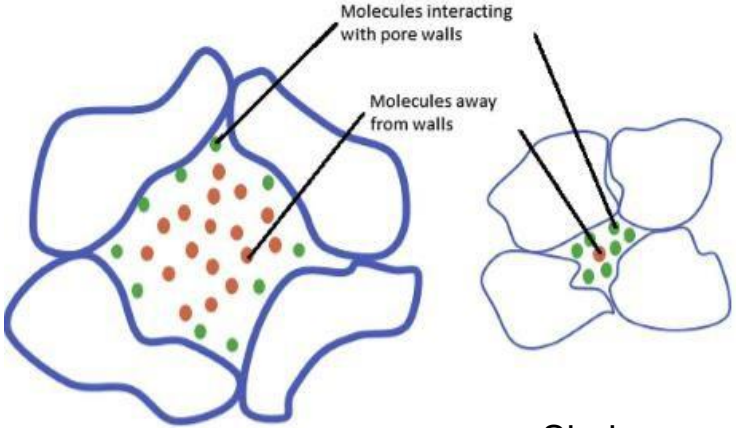
Adsorption & Confinement effects

- **Adsorption Applications:**
  - CO_2 capture (e.g., power plant exhaust gases)
  - Gas Masks
  - Fuel Cells

- **Nanopores**
  - ~80% of shale pores are less than 50 nm.
  - Under confinement, fluid properties significantly deviate from bulk properties.
  - Accumulated production can be drastically improved if matrix processes can be accelerated

Desiccant

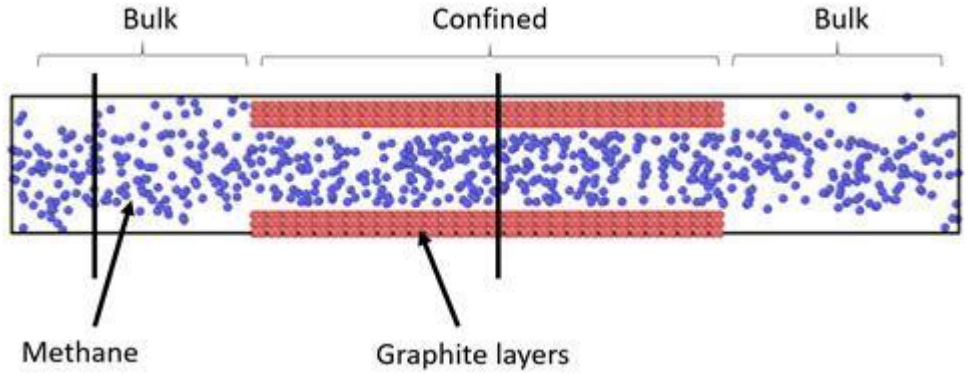

Shale Reservoirs



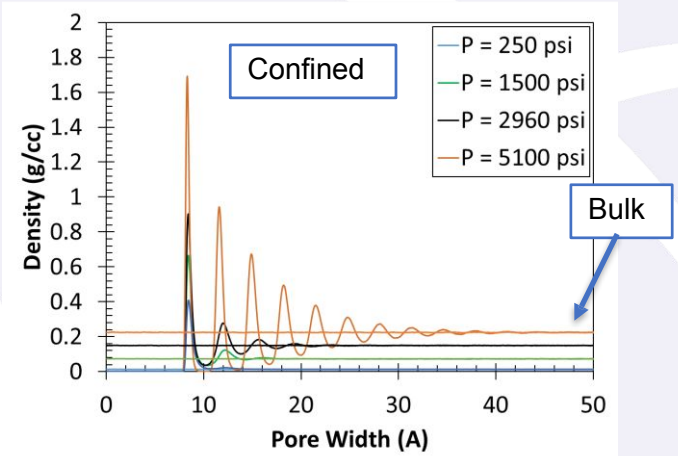
Conventional pore

Shale pore

Adsorption profile in shale pores



Density Profile Cross-section



Density profile of methane in a graphite slit pore

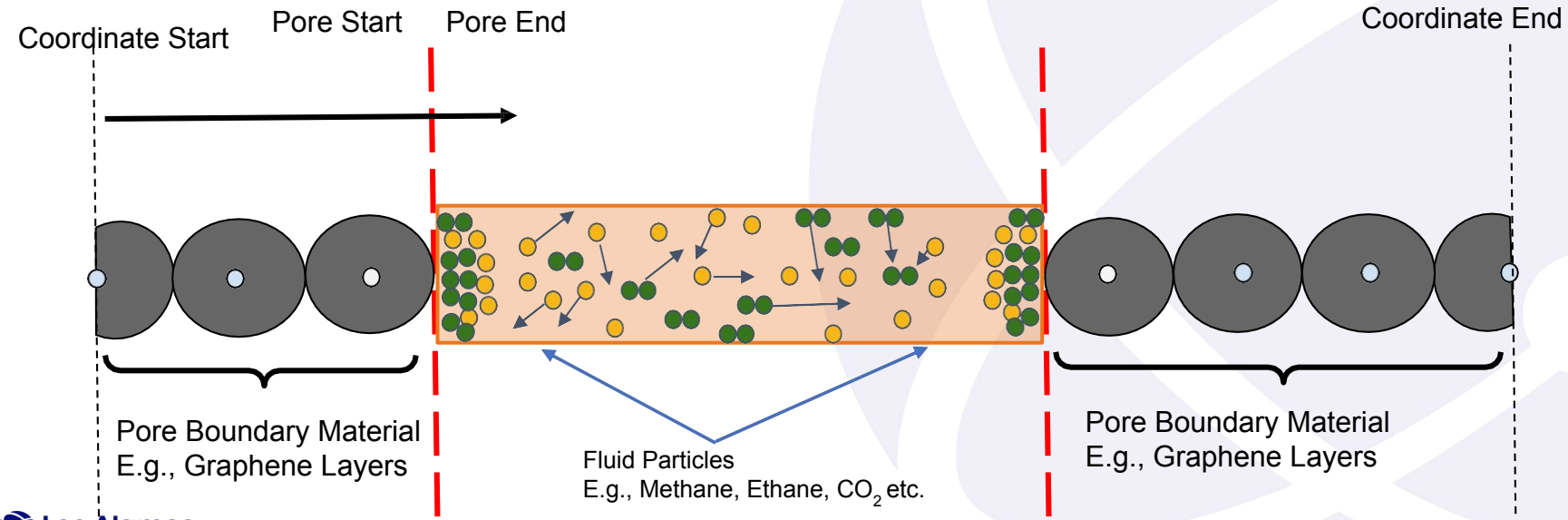
Adsorbed fluid density is ~ 4 times the bulk fluid density

Mehana et al., 2020

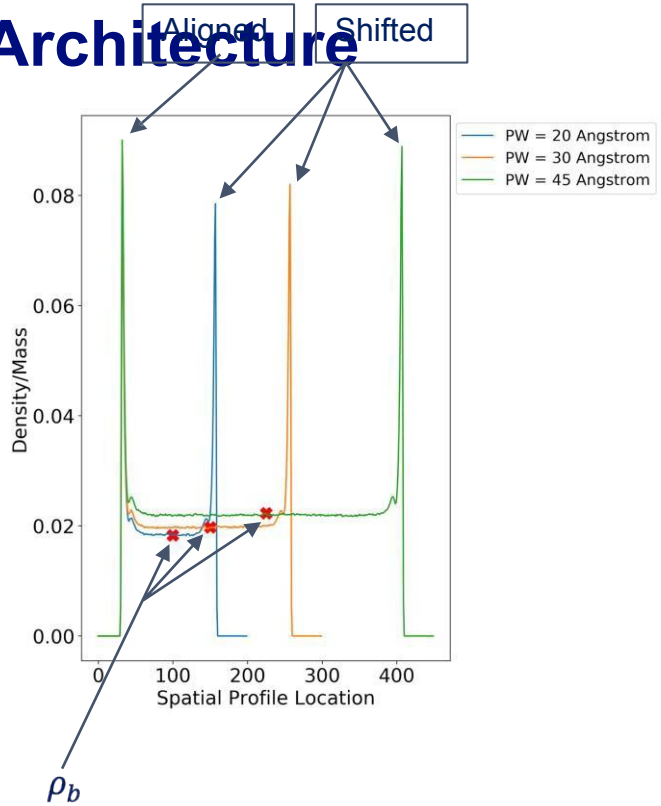
Problem Background & Formulation

- Molecular Dynamics (MD) Simulations can explicitly account for adsorption effects but are expensive

- **Goal**: *Given* an MD setting
  S = {Pore Width,(Angstrom), Pressure(Atmosphere), Temperature(K), Wall Material, Fluid Composition}
  Design an ML solution capable of emulating the MD density profile for a particular experimental setting S



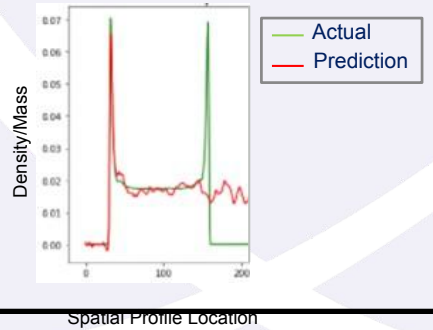
Domain Informed Model Architecture



- ❑ Shift Invariant
- ❑ Decomposed Density Profile Prediction
  - Awareness of ρ_b , adsorption effect
- ❑ Fully Periodic
- ❑ Large Kernel size to capture scale of adsorption effects i.e., large receptive fields

Learnings

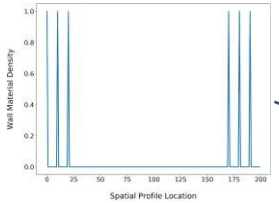
- Need for Shift Invariance
- Example Architecture with FCN and Striding
- Both adversely affect shift-invariance [Chaman et al. 2020]



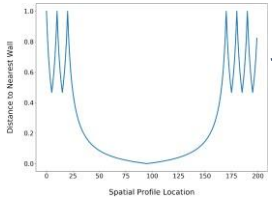
Multi-Task Convolutional Model

TRANSFORM SPATIAL LOCATION TO DENSITY PROFILE

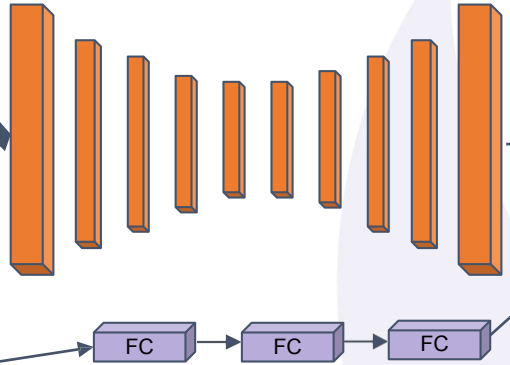
Wall Material Density & Location



Relative Distance to Nearest Wall



[Pressure,Temperature]



$\hat{\rho}_s$

$\hat{\rho}_b$

Dimensions =

$$\hat{\rho}_s \in \mathbb{R}^{1\times l}$$
$$\hat{\rho}_b \in \mathbb{R}^{1\times 1}$$

$$\hat{\rho} = \hat{\rho}_s + \hat{\rho}_b$$

Multi-Task Loss

$$L(\theta) = ||\hat{\rho} - \rho||_2^2 + ||\hat{\rho}_b - \rho_b||_2^2 + \lambda R(\theta)$$

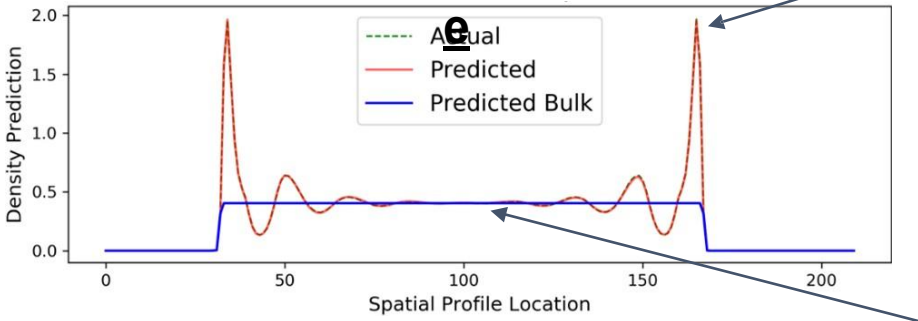
Predicted Density Profile

Predicted Bulk Density

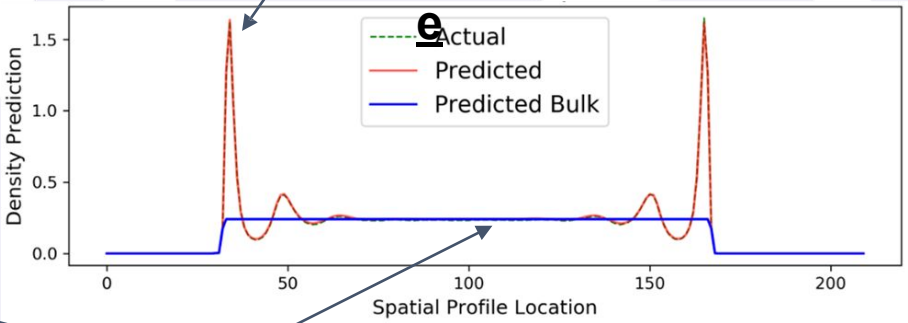
Qualitative Prediction Characterization

Pore Width:
21 Angstrom

Ethane



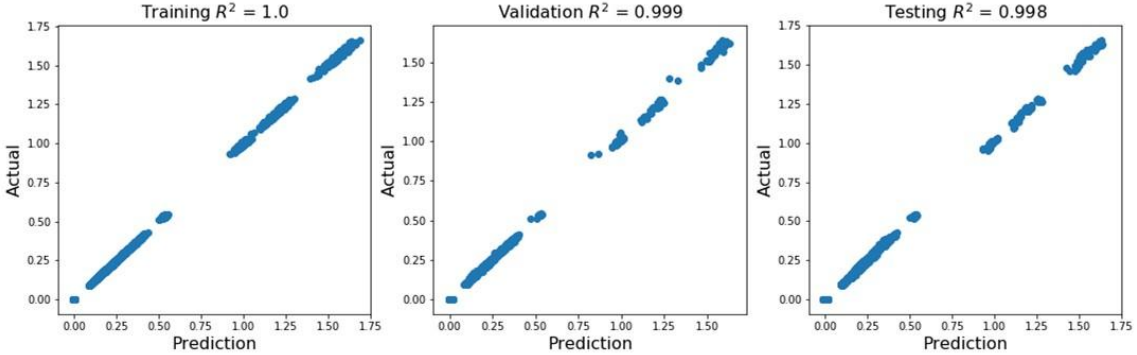
Methane



Different Peak Scales

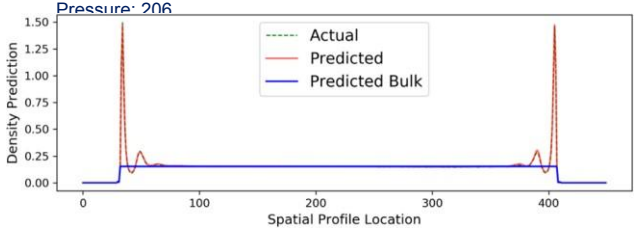
Different Bulk Scales

Performance Characterization (Methane)

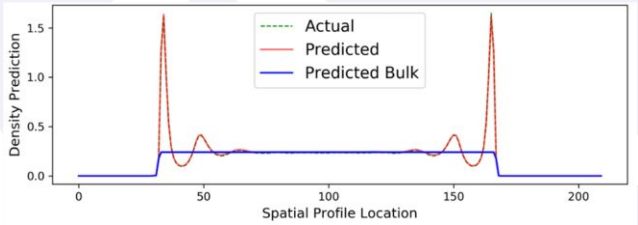


Qualitative Predictions

Experimental Setup:
Pore Width: 45 Angstrom
Temperature: 334 K
Pressure: 206

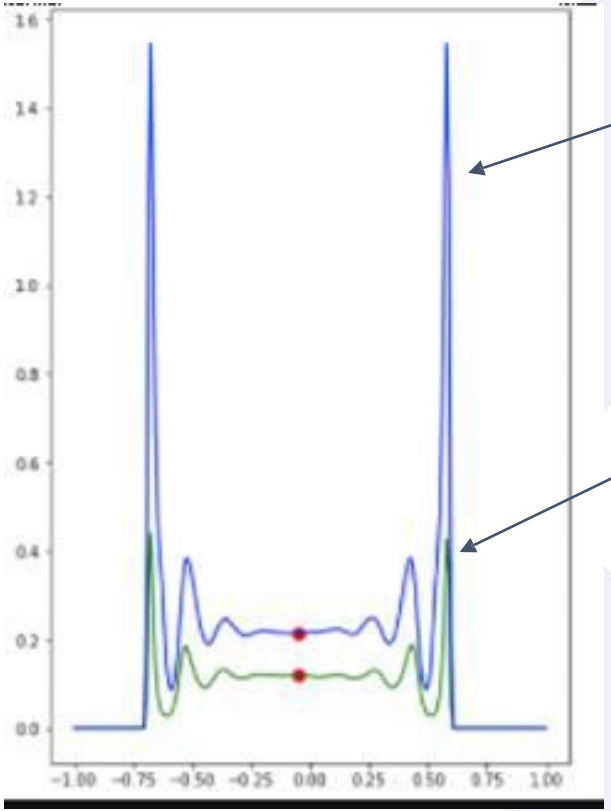


Experimental Setup:
Pore Width: 21 Angstrom
Temperature: 336 K
Pressure: 494



Fluid Mixtures

Sample Density Profile Characterization



Ethane

Methane

Multi-Task Convolutional Model (Fluid Mixture)

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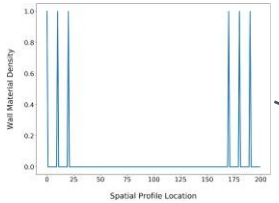
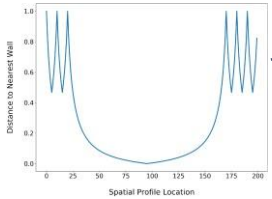
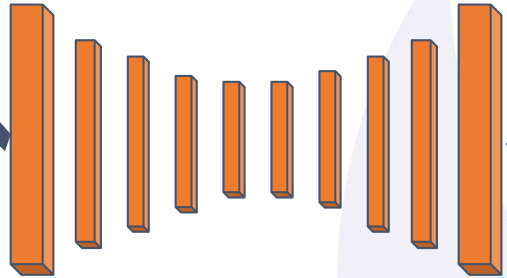


Relative Distance to Nearest Wall



$[pressure, tempearture]$



FC → FC → FC

$\hat{\rho}_s$

$\hat{\rho}_b$

$$\hat{\rho}_{\mathbf{s}} \in \mathbb{R}^{|F| \times l}$$
$$\hat{\rho}_{\mathbf{b}} \in \mathbb{R}^{|F| \times 1}$$

$$\hat{\rho} = \hat{\rho}_s + \hat{\rho}_b$$

Multi-Task Loss

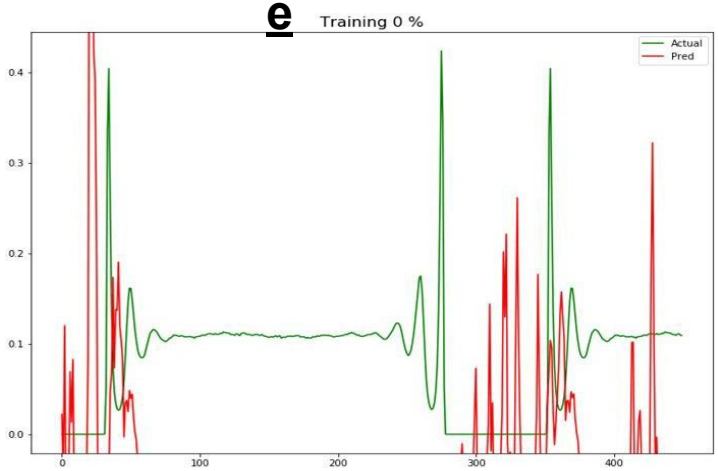
$$L(\theta) = ||\hat{\rho} - \rho||_2^2 + ||\hat{\rho}_b - \rho_b||_2^2 + \lambda R(\theta)$$

Predicted Density Profile

Predicted Bulk Density

Learning Dynamics

Methane

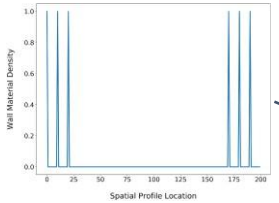


Ethane

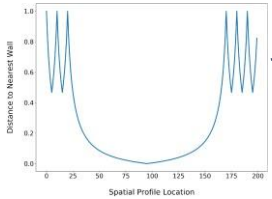
Weighted Multi-Task Convolutional Model (Fluid Mixture)

TRANSFORM SPATIAL LOCATION TO DENSITY PROFILE

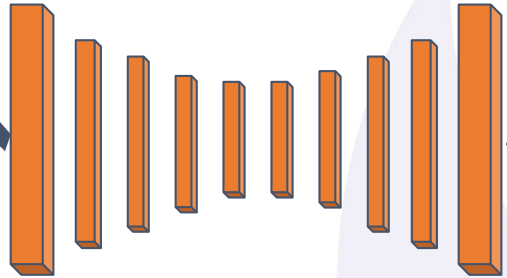
Wall Material Density & Location



Relative Distance to Nearest Wall



$[pressure, tempearture]$



FC → FC → FC

$\hat{\rho}_s$

$\hat{\rho}_b$

$$\hat{\rho} = \hat{\rho}_{\mathbf{s}} \odot \hat{\rho}_{\mathbf{b}}$$

$$\hat{\rho}_{\mathbf{s}} \in \mathbb{R}^{|F| \times l}$$
$$\hat{\rho}_{\mathbf{b}} \in \mathbb{R}^{|F| \times 1}$$

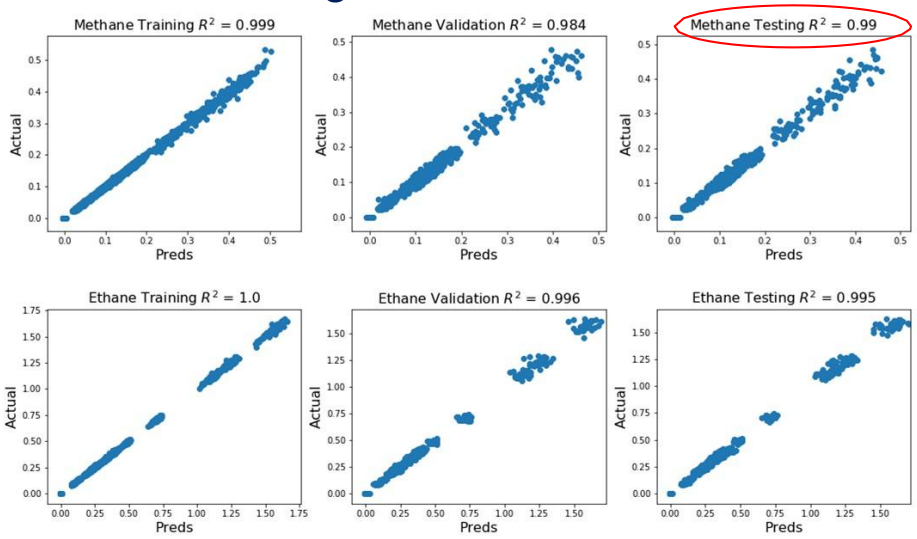
Weighted Multi-Task Loss

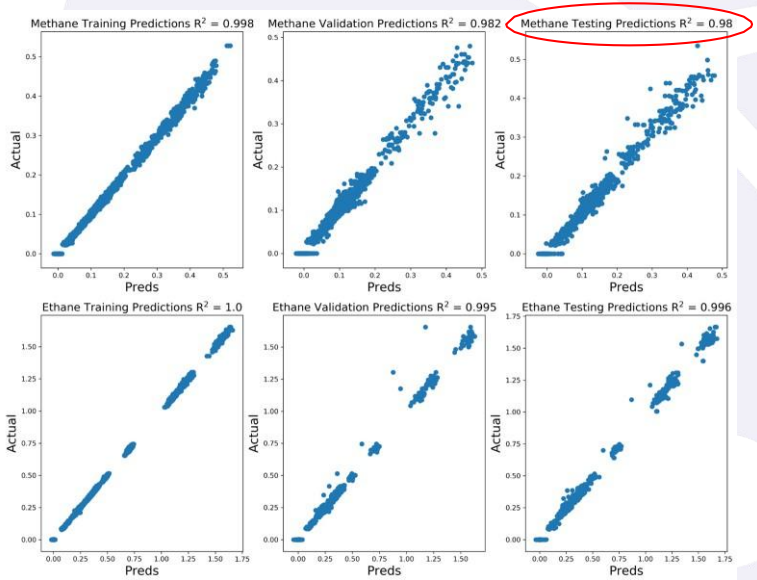
$$L(\theta) = \sum_{i=1}^{|F|} \frac{1}{w_i} ||\hat{\rho}_i - \rho_i||_2^2 + \frac{1}{w_i} ||\hat{\rho}_{bi} - \rho_{bi}||_2^2 + \lambda R(\theta)$$

$$w_i = \rho_{bi}^2 + \sum_{j \in F \setminus f_i} \rho_{bj} \rho_{bi}$$

Fluid Mixture Prediction Performance
Methane-Ethane Fluid Mixture

Weighted Multi-Task CNN Multi-Task CNN

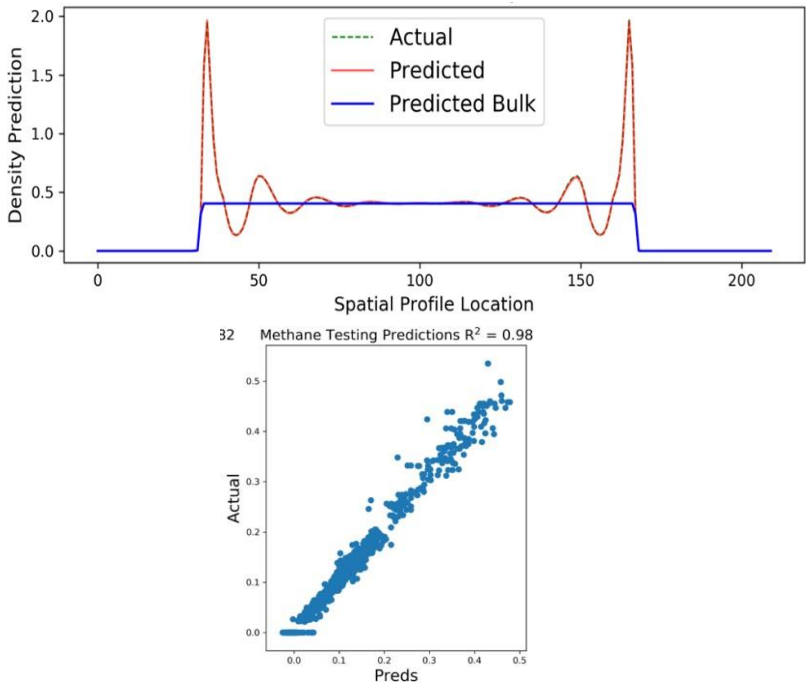




Summary

- Machine Learning based **MD emulator** capable of generating density profiles for unseen conditions
  - Domain informed fully convolutional solution
- (Weighted) Multi-Task CNN Model to handle **Single Fluids** & **Mixtures**
  Results on Single & Multiple fluids indicate **promising initial results**
- Future Work
  - Fully Periodic Convolutional Network
    Smoother Adsorption Isotherm
  - Few-shot generalization
  - Novel Mixtures (i.e., unseen fluids)
    Novel Wall-Material (affects adsorption properties)
    Method: Meta-learning

Data-driven Models of Adsorption Equilibria of Multi-component Mixtures in Porous Materials



Machine learning vs molecular simulations predictions for single and multi-component systems

Project Description

We propose building machine learning capabilities to develop adsorption models for multi-component systems of interests to subsurface applications using a molecular- simulation-generated database.

Project Outcomes:

Develop fast and reliable data-driven models to predict the adsorption characteristics of multi- component mixtures of interest to subsurface applications.

PI: Mohamed Mehana
Total Project Budget: $40k
ISTI Focus Area: Data Science and Artificial Intelligence

Los Alamos NATIONAL LABORATORY

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