Rapid and Accurate Prediction of CO2 Adsorption Performance Using Deep Learning Model

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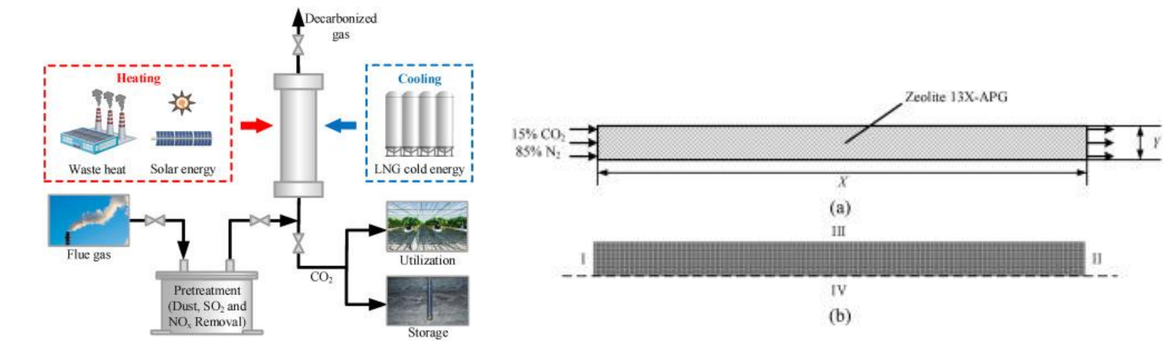
Introduction

- **Open adsorption system for atmospheric CO2**



The global challenge of greenhouse gas emissions has identified carbon dioxide adsorption technology as one of the key solutions. This process is characterized by complex mechanisms of heat and mass transfer, alongside dynamic spatiotemporal characteristics that demand extensive computational resources.

- **Deep Learning in CFD**

Recent studies have already demonstrated the application of deep learning in the field of Computational Fluid Dynamics (CFD) for two-dimensional field data through data-driven approaches, achieving an approximate thousandfold increase in computational speed. However, these methodologies are still constrained by their ability to predict only a singular type of data.

Stender,,et al. U^p-Net: a generic deep learning-based time stepper for parameterized spatio-temporal dynamics. Comput Mech 71, 1227–1249 (2023).

This study introduces a deep learning-based approach designed to harness the power of limited available data for the rapid and precise prediction of carbon dioxide adsorption capabilities under varying conditions. Specifically, it employs deep learning techniques to concurrently predict multiple types of two-dimensional field data (such as pressure and adsorption quantity) within the same operational scenario.

Method

- **CFD Model:**

Mass equation

$$\frac{\partial(\varepsilon\rho)}{\partial t}+\mathrm{div}(\rho\vec{v})=-(1-\varepsilon)\rho_s\sum_i M_i\frac{\partial q_i}{\partial t}$$

Momentum equation

$$\frac{\partial(\rho\vec{v}/\varepsilon)}{\partial t}+\mathrm{div}(\rho\vec{v}\vec{v}/\varepsilon^2)=-\mathrm{grad}P+\mathrm{div}(\vec{\tau})-\left[A\frac{(1-\varepsilon)^2\mu}{\varepsilon^3 d_p^2}\vec{v}+B\frac{1-\varepsilon}{\varepsilon^3 d_p}\rho|\vec{v}|\vec{v}\right]$$

viscous and inertial resistances.

Energy equation

$$\frac{\partial\left(\varepsilon\rho E+(1-\varepsilon)\rho_s E_s\right)}{\partial t}+\mathrm{div}\left(\vec{v}(\rho E+P)\right)=\mathrm{div}\left[k_{eff}\,\mathrm{grad}\,T-\sum_i h_i\vec{J}_i+\tau\vec{v}\right]+(1-\varepsilon)\rho_s\sum_i-\Delta H_i\frac{\partial q_i}{\partial t}$$

Xuetao Liu, et al., Open adsorption system for atmospheric CO2 capture: Scaling and sensitivity analysis,Energy,Volume 294,2024,130805,ISSN 0360-5442.

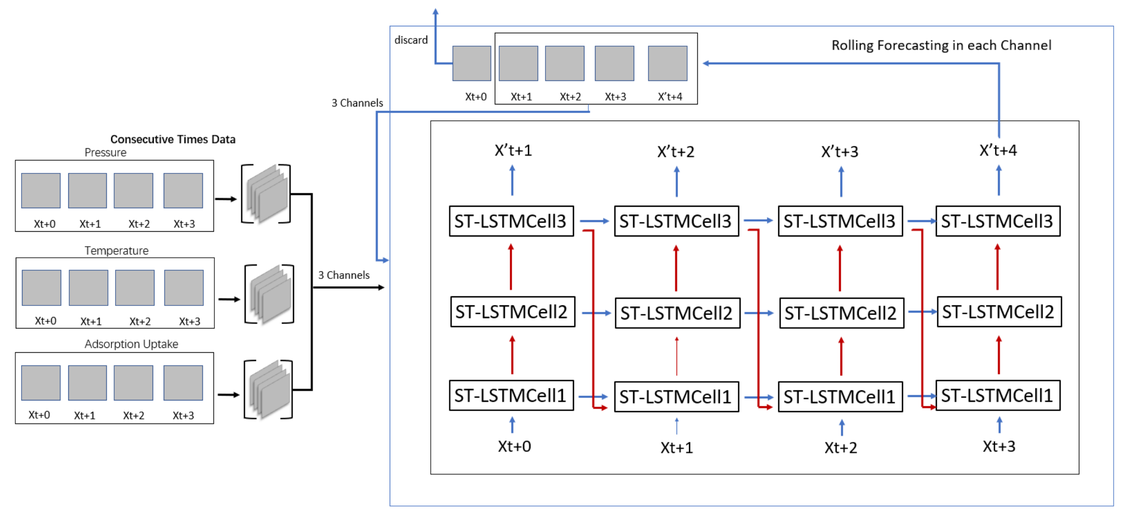
- **Data Generation:**

We employed seven different operational conditions, encompassing a variety of inlet velocities and adsorption thermal conductivity coefficients. Through the application of rotation and flipping operations, we generated a total of 59,880 data sets for model training and 9,980 data sets for model validation.

- **Spatiotemporal Prediction:**

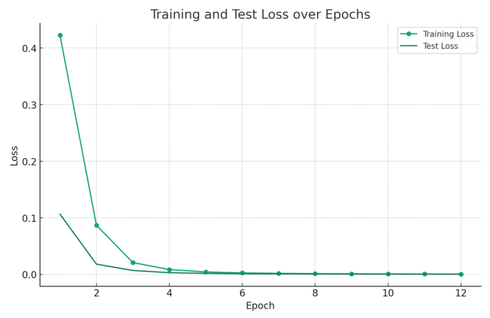
The method of prediction by the model is illustrated in the figure below. The left side of the figure displays different two-dimensional field data, including variables such as pressure, temperature, and adsorption uptake. In our research, the data from the first four time steps are used as a time series, which forms a time channel for the model, while pressure, temperature, and adsorption uptake form the data category channels. These three data categories and their corresponding time series are input in parallel into the PredRNN model. The PredRNN model is capable of capturing spatio-temporal features at each time point based on the input time series. These features not only propagate within the same layer of the model but also communicate between different layers, with each layer outputting the prediction results for the current time point. In the prediction phase, only the prediction result of the last time point is used as the final output. This output is then reintegrated into the input time series as new input data, while the first time point of the original time series is discarded. This prediction strategy is referred to as rolling forecasting.

Method



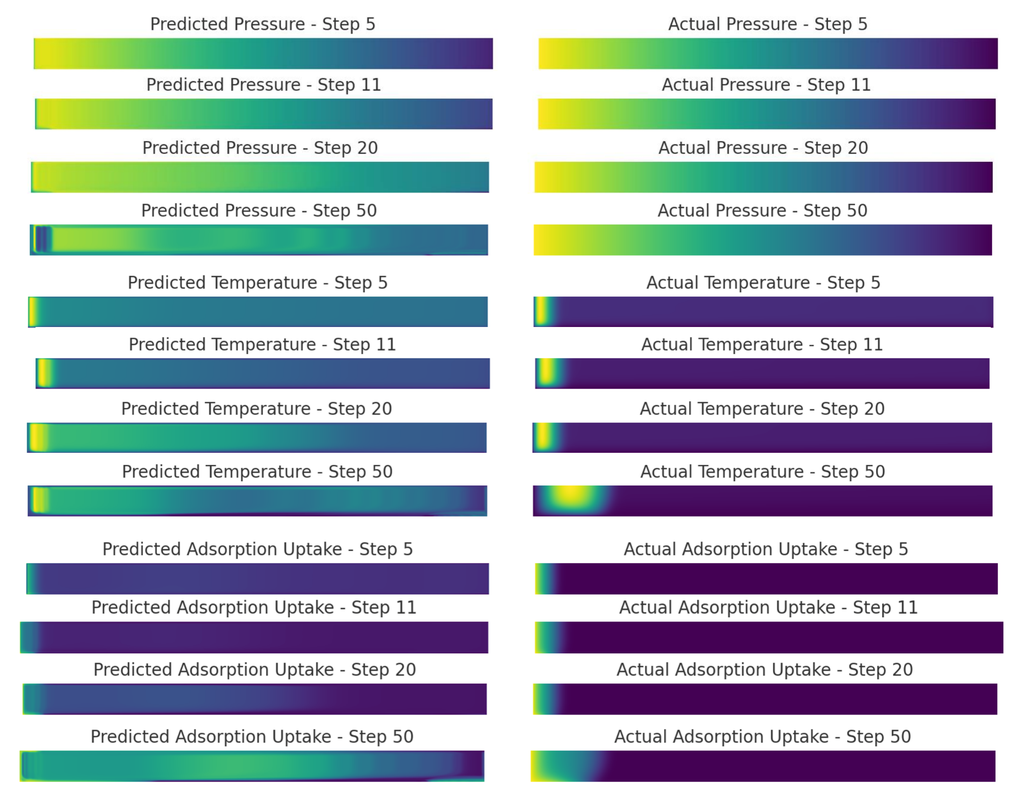
Results

The PredRNN model underwent approximately 50 hours of training on an RTX 4080 GPU. The duration for each prediction step is approximately 0.038s.



Time Step	MSE	MAE	
5	0.4033	0.2494	0.999979
20	18.3684	2.2276	0.999056
50	116.7551	6.8205	0.994086

The table displays the predictive performance of the PredRNN model for three types of data: pressure, temperature, and adsorption uptake. As the time steps increase, the model's predictive errors, reflected by the Mean Squared Error (MSE) and the Mean Absolute Error (MAE), also rise, while the coefficient of determination (R2) experiences a slight decline.



As illustrated in the figure, there is a gradual accumulation of error with the stepwise increment, ultimately resulting in a significant deviation of the predicted values from the actual data. This discrepancy with the model's performance at corresponding time steps underscores the necessity for refinement in the training process, particularly an adjustment of the loss function.

Future Work

- Optimize model parameters to enhance predictive precision.
- Refine training techniques to bolster model learning efficacy.
- Adjust the loss function to mitigate the cumulative error associated with incremental time steps.
- Investigate novel deep learning frameworks for handling two-dimensional temporal series data (feature decomposition strategies).