

A Deep Learning Modeling Framework to Capture Mixing Patterns in Reactive-Transport Systems

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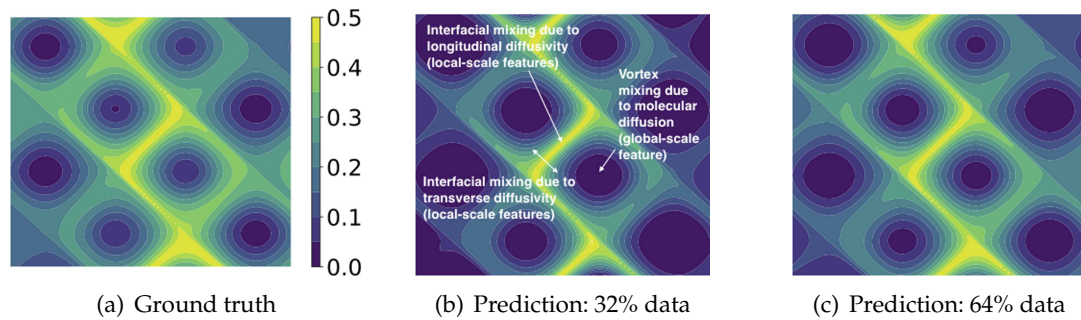
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Abstract. Prediction and control of chemical mixing are vital for many scientific areas such as subsurface reactive transport, climate modeling, combustion, epidemiology, and pharmacology. Due to the complex nature of mixing in heterogeneous and anisotropic media, the mathematical models related to this phenomenon are not analytically tractable. Numerical simulations often provide a viable route to predict chemical mixing accurately. However, contemporary modeling approaches for mixing cannot utilize available spatial-temporal data to improve the accuracy of the future prediction and can be compute-intensive, especially when the spatial domain is large and for long-term temporal predictions. To address this knowledge gap, we will present in this paper a deep learning (DL) modeling framework applied to predict the progress of chemical mixing under fast bimolecular reactions. This framework uses convolutional neural networks (CNN) for capturing spatial patterns and long short-term memory (LSTM) networks for forecasting temporal variations in mixing. By careful design of the framework—placement of non-negative constraint on the weights of the CNN and the selection of activation function, the framework ensures non-negativity of the chemical species at all spatial points and for all times. Our DL-based framework is fast, accurate, and requires minimal data for training. The time needed to obtain a forecast using the model is a fraction ($\approx \mathcal{O}(10^{-6})$) of the time needed to obtain the result using a high-fidelity simulation. To achieve an error of 10% (measured using the infinity norm) for capturing local-scale mixing features such as interfacial mixing, only 24% to 32% of the sequence data for model training is required. To achieve the same level of accuracy for capturing global-scale mixing features, the sequence data required for model training is 64% to 70% of the total spatial-temporal data. Hence, the proposed approach—a fast and accurate way to forecast long-time spatial-temporal mixing patterns in heterogeneous and anisotropic media—will be a valuable tool for modeling reactive-transport in a wide range of applications.

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The images in this figure compare the ground truth (left) and the predictions (middle and right) from the proposed framework at the end of the simulation (i.e., time = 1.0). The middle image is a forecast based on training using the first 32% of input data; training data is provided until $t = 0.32$ and the model predicts for the rest of the simulation time. Likewise, the right image provides the forecast based on the 64% of the input data. For capturing local-scale mixing features (e.g., interfacial mixing due to anisotropy), 32% input data will suffice to make predictions within 10% error. In addition, to capture global-scale mixing features (e.g., mixing near vortices caused by molecular diffusion) with similar accuracy, one will need approximately twice the amount of data.

Abbreviations

CNN: Convolutional Neural Network,
 DL: Deep Learning,
 FEM: Finite Element Method,
 LSTM: Long Short-Term Memory,
 RNN: Recurrent Neural Network

1 Introduction and motivation

Reactive-transport equations arise in a wide range of scientific domains like epidemiology [53], combustion [41], hypersonic flows [26, 45, 46, 56], subsurface energy [55], contamination remediation [9], air and water quality research [58], and population dynamics [42]. Although the underlying mathematical models in these applications are similar, the associated spatial and temporal scales are much different. For example, the spatial domains in combustion and hypersonic flows are small: an internal-combustion engine for