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Towards Digital Twins of Capillary Mass Diffusion Experiments: A Physics-based Machine-Learning Framework for Inverse Modeling of Mass Transport Processes

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Digital twins of experiments are increasingly realistic numerical models that enhance experimental observations by closely simulating real-world phenomena and offering insights into complex processes and can support the measurement of specific quantities via inverse modeling by adjusting model parameters to match observed data, thus refining our understanding of the underlying mechanisms. For inverse modeling, numerous high-fidelity, three-dimensional simulations are required, which are typically extremely time-consuming. To overcome this computational hurdle and enable real-time analysis, we have developed a physics-based machine learning (ML) framework that utilizes trained neural networks for rapid predictions, significantly speeding up the overall process by efficiently approximating complex calculations. The application of this approach is illustrated in the mass diffusion experiment, which involves two reservoirs connected by a capillary tube filled with high-porosity porous media. This experimental setup permits non-destructive in-situ chemical imaging through fluorescence measurements at the Swiss Light Source (SLS, Paul Scherrer Institute), allowing for the monitoring of the two-diemnsional distribution of local chemical species concentrations throughout the capillary at multiple time points. Inverse modeling is conducted using the trained ML model, with the implementation of several global optimization techniques. The framework has been validated against synthetic concentration profiles and has been applied to actual experimental data to estimate the parameters of interest. The total time cost for developing such a framework, after having the first numerical model of the experiment and access to the necessary computational resources (including dataset generation, training, and the optimization process), was less than 15 hours in this case, which is shorter than the 130 hours required to perform one actual experiment. A key benefit of this framework is its capacity for immediate output generation for exploring the effect of different controlling parameters, including the effective diffusion coefficient and temporal instances, providing a shortcut to the extensive and expensive recalculations required by full physical simulations. Extensions to experiments involving carbonate precipitation will also be discussed.