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Deep learning to predict the effectiveness factor in the closure problems EHSAN TAGHIZADEH, Oregon State University, PAUL MACKLIN, Indiana University, HELEN BYRNE, University of Oxford, BRIAN WOOD, Oregon State University — We adopt a combination of upscaling and machine learning to generate a closed macroscale equation to predict convection, diffusion, and reactions within a tissue. We start with a microscale description of the system. We upscale these equations to determine a macroscale representation of the system. Nonlinearity in the reaction rate prevents computation of the closure factor using conventional analytical techniques. We overcome the nonlinear closure problem by using deep neural networks (DNNs) to learn an appropriate representation. First, we construct a simple representative geometry, that approximates the true geometry. Then we determine the features space on the basis of the source terms in the nonlinear closure problem. Next, we perform exhaustive microscale simulations for the nonlinear problem to compute an effectiveness factor at each point in feature space. Then, we design a DNN that learns the nonlinear dependencies from the features space. Finally, we test the algorithm on two representative tissues (brain and liver) with different cell geometries and scales. Our results show that the effectiveness factor predicted from the artificial neural network can accurately estimate the correction factor computed by the direct numerical solutions.

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