# A surrogate model for $CO_2$ methanation in an isothermal fixed-bed reactor using physics-informed neural network

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This study presents a physics-informed neural network (PINN) surrogate model (SM) for $CO_2$ methanation in an isothermal fixed-bed reactor (IFB). Unlike common SMs, PINN implicated physics terms including governing equations, boundary conditions, initial conditions, and reaction kinetics during training the network parameters. The strategy for tunning ANN hyper-parameters such as number of hidden layers and neurons, activation functions, number of collocation training points, and training data range was discussed. In the PINN forward problem, the extrapolation capability of SM for the plug-flow reactor model for IFB was examined. The outstanding extrapolation capability of PINN was proven by an exellent prediction for the testing result from more than 10 times out of the training data range. In the PINN inverse problem, an unknown IFB model parameter such as effectiveness factor was estimated with a prediction accuracy of 98.8% using just 20 data points. PINN showed a great potential in building SMs for chemical reactor design and revealing model parameters of chemical reaction kinetics.