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Accelerating models for multiphase chemical kinetics through machine learning with polynomial chaos expansion and neural networks

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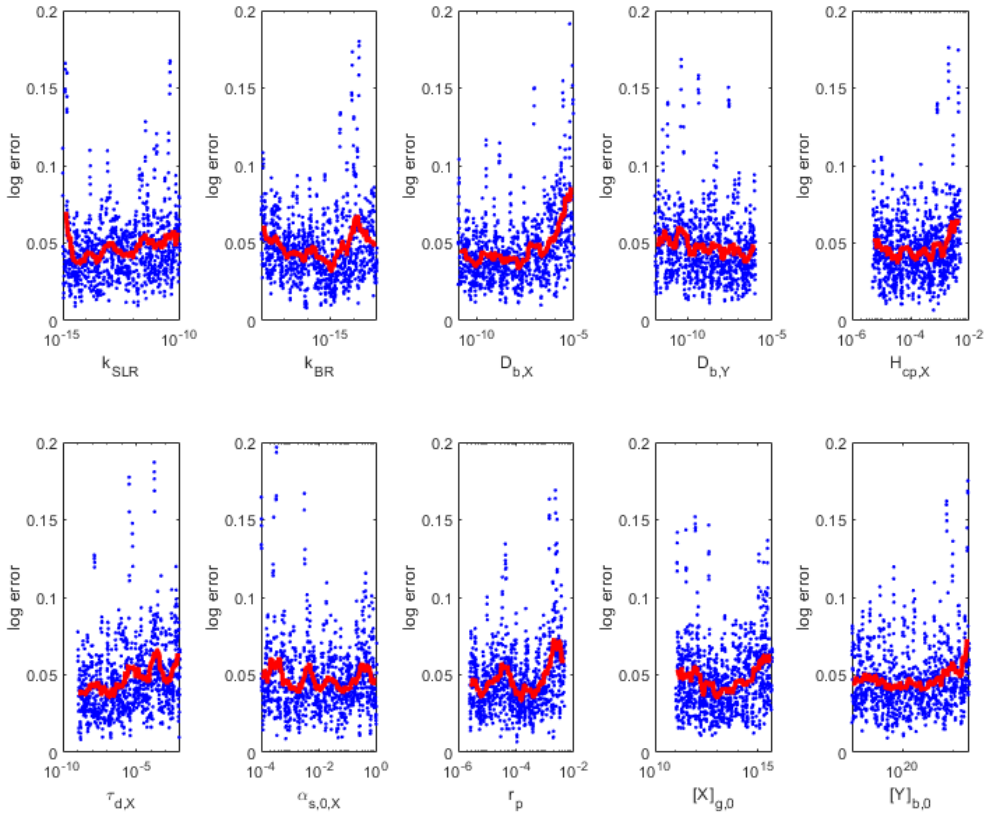

Figure S1. Absolute logarithmic error of the surrogate model for the 50 % reaction time (chemical half-life) in the test data set (N=1000) as a function of all 10 model input parameters. Due to the large size of the test data set and the variability in model error, errors are depicted as moving averages between the n=5 (blue dots) and n=100 (red lines) closest neighbours in a sorted list with ascending parameter values, respectively. No significant dependence of surrogate model error on parameter values is observed.