Predictive Analytics And Uncertainty Quantification Of A Microscale Porous Reactor Simulation

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Abstract

The use of computer simulations to analyze systems during the design process is a popular approach for validating and optimizing designs. But simulations are deterministic in nature and do not consider the uncertainty in design, manufacturing, and use of the product. Using predictive analytics and uncertainty quantification, engineers and data scientists can predict the range of possible outcomes for a given design accounting for such uncertainties. By building predictive models of simulations, engineers and data scientists can efficiently perform advanced analytics and obtain new insights.

Using a COMSOL® simulation of a microscale porous reactor, this presentation will provide an example of the above uses of predictive analytics and uncertainty quantification. Topics to be discussed will begin with the creation and use of Design of Experiment to select the best COMSOL® simulations to run for predictive model training data acquisition. Results will include an optimization of design parameters using the predictive model of the COMSOL® simulation and the propagation of uncertainties around the optimized solution.