Validity domain constrained hybrid modeling of fed-batch reactor system for optimization of input strategy

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With ongoing advances in sensor technology, massive amounts of operational data are becoming available for industrial processes. In this situation, a framework combining first principles and data-based models to describe systems with unknown kinetics can be a remedy to the problems in the field of process modeling. This study proposes a hybrid modeling approach that combines a first principles model with deep neural networks (DNN) that can utilize complex process data and capture dynamic behaviors of unknown or poorly known kinetics of a reactor system. It is also important to identify effective range for the model prediction if the hybrid model is to be used for other tasks such as optimization. The proposed approach includes criteria for checking "valid domain" of the hybrid model to assess whether the prediction is from undue extrapolation or not. The criteria are represented as convex hull and confidence interval so that they can be readily integrated into dynamic optimization as sets of linear inequality constraints. As an illustration of industrial operations, feed-rate optimization of a fed-batch reactor will be presented and show the efficacy of the proposed scheme.