Quantifying the impact of temporal analysis of products reactor initial state uncertainties on kinetic parameters

Adam Yonge[1], M. Kunz[2], Gabriel Gusmão[1], Zongtang Fang[2], Rakesh Batchu[2], Rebecca Fushimi[2], and Andrew Medford[1]

[1]Georgia Institute of Technology
[2]Idaho National Laboratory

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Abstract

The temporal analysis of products (TAP) reactor provides a route to extract intrinsic kinetics from transient measurements. Current TAP uncertainty quantification only considers the experimental noise present in the outlet flow signal. Additional sources of uncertainty such as initial surface coverages, catalyst zone location, inert void fraction, gas pulse intensity and pulse delay, are not included. For this reason, a framework for quantifying initial state uncertainties present in TAP experiments is presented and applied to a carbon monoxide oxidation case study. Two methods for quantifying these sources of uncertainty are introduced. The first utilizes initial state sensitivities to approximate the parameter variances and provide insights into the structural certainty of the model. The second generates parameter confidence distributions through an ensemble-based sampling algorithm. The initial state covariance matrix can ultimately be merged with the experimental noise covariance matrix, providing a unified description of the parameter uncertainties for a TAP experiment.

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