(185t) Multi-Scale Simultaneous Parameter Estimation in Rate-Based Processes

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Unbiased and consistent
estimation of model parameters using noisy experimental data is an essential requirement for developing predictive models. While there has been considerable progress in this area in the last few decades, optimal estimation of model parameters is still challenging for reactive solvent-based processes. Simultaneous mass and heat transfer coupled with fast chemical reactions that cannot be distinguished from each other make the parameter estimation problem for these systems considerably more difficult. The typical approach in the literature to circumvent this problem is to develop these models sequentially by designing experiments that attempt to isolate a specific mechanism. For example, a diffusivity model is first developed considering a surrogate system where no reaction takes place. Then, data from a bench scale wetted wall column (WWC) is used to develop models for the mass transfer coefficients and reaction kinetics, where the previously established diffusivity model is assumed to be

valid. Finally, an interfacial area model is developed for a given packing based on pilot scale absorber and regenerator data. Another approach is to obtain the mass transfer coefficient model using experimental data from a nonreactive system in the packed tower. Then data for the actual, reactive system can be used to develop the interfacial area submodel.

The traditional sequential approach implicitly assumes that the diffusivity and mass transfer coefficient models obtained from different types of equipment are valid for each type of equipment and system (e.g., that the WWC column and non-reactive system are valid for the reactive system in a packed column). However, the hydrodynamics, liquid and gas velocities, loading of the solvent and operating temperatures can be very different. Also, significant differences in density, viscosity, and surface tension between the reactive and non-reactive systems can affect the wettability and flow characteristics of the fluids, hence the interfacial area. Furthermore, the mass transfer for electrolyte systems is affected by the ionic species present in the solution, ion-molecule interactions, and ion mobility. Therefore, the parameters that are estimated for a given scale or a surrogate system may not be necessarily optimal for the system. Thus, the error in parameter estimation from one step gets propagated to the next step.

In this work, a novel simultaneous parameter estimation technique is developed where parameters for mass transfer, diffusivity, interfacial area, and reaction kinetics are optimally estimated leveraging noisy, experimental data from multiple scales (mm-scale to m-scale) and operating conditions using high-fidelity process models (Chinen et al., 2018). The proposed approach leads to a large-scale optimization problem consisting of a large number of parameters and millions of linear and nonlinear equality and inequality constraints. The optimization problem is solved using the Institute for the Design of Advanced Energy Systems' (IDAES) computational framework that facilitates large-scale parameter estimation at multiple scales embedded in complex process models and property submodels while utilizing data from various sources and scales (Eslick et al., 2018). The software platform provides modular process modeling capabilities using the Pyomo algebraic modeling language (Hart et al., 2011) and the PySP module in Pyomo for stochastic programming and parameter estimation (Watson et al., 2012). Our previous work focused on the parameter estimation problem for a MEA-H_2O-CO_2 system where the data from the WWC and pilot plant were used (Eslick et al., 2018). The Non-random-two-liquid (NRTL) model was implemented to model the vapor-liquid equilibrium at the interface of

the liquid/gas films. Even though the WWC and packed tower models were rigorous in that work, a simple mass transfer model was used to describe the CO_2 and H_2O transport across the liquid and gas films. In particular, it was assumed that the change in the concentration driving force is linear across the films. Chemical reactions in the liquid film were not explicitly considered in that model, rather an enhancement factor was used to capture the enhancement in mass transfer due to the chemical reactions. However, due to the fast ionic reactions in the liquid film of the MEA-H_2O-CO_2 system, complex thermodynamics of this electrolyte system, and interactions between the molecular and ionic species, the CO_2 concentration profile in the liquid film is highly nonlinear. Therefore, the parameter estimates under linear assumption can be inaccurate. In the updated model, simultaneous mass transfer and chemical reactions are considered in the liquid film. Multicomponent mass transfer in the liquid and gas films is modeled by the Maxwell-Stefan equations.
Furthermore, a rigorous electrolyte NRTL model is implemented to model the vapor-liquid equilibrium at the interface of the liquid/gas films. Experimental data sets are also expanded to include the data from the WWC, bench-scale, and pilot-scale systems extending the richness of the experimental data considerably. These modifications increased the size of the optimization problem substantially. Model reformulations are carried out and novel solution strategies are developed to solve the parameter estimation problem within reasonable time. Various approaches investigated in this work includes direct simultaneous optimization, decomposition via PySP and an approach using cross-validation and statistical inference. It is observed that the variance in the parameter estimates can be substantially improved by including the data from multi-scale systems simultaneously.

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