A Comparison of Convergence Reliability for Flowsheet Optimization with First-Principles, Surrogate, and Implicit Formulations of a Gibbs Reactor

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Computing optimal operating conditions of a chemical process flowsheet is a fundamental aspect of process design. However, classical optimization of these processes is challenging due to the number of variables and algebraic equations defining each unit operation, as well as the nonlinear complexity of these first principles models. Convergence of these optimization models is sensitive to initial guess, scaling, and problem formulation.

To improve solver convergence reliability when optimizing a chemical process flowsheet, we implement two alternative approaches. First, data-driven optimization based on surrogate modeling. This approach relies on representing complex thermodynamics and chemical reaction equations with tractable and simple polynomials with reduced dimensionality. Second, an implicit function formulation based on [1]. In this approach, the complex first-principles algebraic equations are converged separately as an implicit function and the resulting values and derivatives are communicated back to the optimization solver.

We aim to optimize the autothermal reforming (ATR) section of a hydrogen manufacturing process. We implement the flowsheet using IDAES-PSE [2], and compare instances with first-principles (or full space), surrogate-based, and implicit function-based models for the reforming reactor..

The full space flowsheet (baseline) is modeled with the first-principles Gibbs Reactor. In the second flowsheet, the Gibbs Reactor is replaced by a surrogate block containing polynomials generated by the ALAMO [3] machine learning framework. Finally, in the third flowsheet, the Gibbs Reactor is replaced by an external implicit function using PyNumero [4]. The optimization problems were solved with IPOPT [5]. We compare convergence reliability, solve time, and solution quality between these three flowsheets.

To demonstrate the potential of surrogate-based and implicit function-based optimization, we solve 64 instances parameterized by inlet natural gas pressure and temperature. Preliminary convergence reliability results are shown in **Figure 1**. The full space formulation was able to converge 38 out of 64 instances in an average of 3.7 s, while the surrogate-based formulation converges all instances in an average of 0.9 s with only a minor increase in solution error. The mean relative error between objective values is 1.5%. The implicit function-based formulation converged 53 of these instances in an average of 34 s, with no solution error.

A screenshot of a computer

Description automatically generated with low confidence

**Figure 1.** Convergence status for the three formulations.

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