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A framework for efficient large scale equation-oriented flowsheet optimization

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ABSTRACT

Despite the economic benefits of flowsheet optimization, many commercial tools suffer from long computational times, limited problem formulation flexibility and numerical instabilities. In this study, we address these challenges and present a framework for efficient large scale flowsheet optimization. This framework couples advanced process optimization formulations with state-of-the-art algorithms, and includes several notable features such as (1) an optimization-friendly formulation of cubic equation of state thermodynamic models; (2) a new model for distillation column optimization based on rigorous mass, equilibrium, summation and heat (MESH) equations with a variable number of trays that avoids integer variables; (3) improvements on the Duran–Grossmann formulation for simultaneous heat integration and flowsheet optimization; and (4) a systematic initialization procedure based on model refinements and a tailored multi-start algorithm to improve feasibility and identify high quality local solutions.

Capabilities of the framework are demonstrated on a cryogenic air separation unit synthesis study, including two thermally coupled distillation columns and accompanying multistream heat exchangers. A superstructure is formulated that includes several common ASU configurations in literature. As part of the optimization problem the solver selects the best topology in addition to operating conditions (temperatures, flowrates, etc.) for coal oxycombustion applications. The optimization problem includes up to 16,000 variables and 500 degrees of freedom, and predicts specific energy requirement of 0.18 to 0.25 kWh/kg of O_2 depending on design assumptions. These results are compared to literature and plans to extend the framework to an entire coal oxycombustion power plant optimization study are discussed.

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1. Introduction

Flowsheet optimization and synthesis improve process designs by systematically exploring nearly uncountable process configurations. By facilitating the selection of the best designs, optimization ultimately reduces costs, increases efficiency and improves plant operability. Applied to tomorrow's power systems, large scale optimization will help reduce the capital and operational costs of carbon capture, utilization and sequestration. Furthermore, optimization frameworks allow for an automated, systematic screening of promising technologies, ranging from single systems, such as membranes for CO_2 separation, to entire new flowsheets, such as coal oxycombustion. As a result, they provide insight to the potential value of new technologies throughout the development cycle.

Equation oriented (EO) approaches offer several advantages over more traditional sequential modular (SM) methods for simulation. Sequential modular methods work by simulating each unit (module) individually and then converging the entire flowsheet with a combination of iterations and heuristics. In contrast, equation oriented methods apply Newton's method for solving systems of nonlinear equations to simulate the flowsheet, enabling simultaneous optimization and convergence of the flowsheet. More generally, EO formulations directly exploit advances in mathematical programming development, leading to distinct advantages over SM methods with regards to optimization, including:

- **Efficient large scale solvers:** The availability of accurate first and second derivative information calculated via automatic differentiation enables the use of very efficient large scale nonlinear programming algorithms, capable of handling 100,000+ constraints and equations (including inequality constraints). Optimization algorithms available in SM packages (such as SQP

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methods) cannot handle these large problems and typically experience convergence difficulties due to inaccurate derivative information. Alternately derivative free methods (genetic algorithms, particle swarm, etc.) are commonly used with SM approaches. These algorithms, however, are less efficient and may not provide guarantees that their results are optimum.

- **Modeling discrete events and decisions:** Many process synthesis tasks require modeling discrete events and decisions. These can be accommodated in EO frameworks with disjunctive programming and mixed integer nonlinear programming (MINLP) algorithms. Furthermore, some discrete variables can be replaced with smoothing functions or complementarities (Dowling and Biegler, 2013; Kraemer et al., 2009; Stein et al., 2004), another active area of mathematical programming research. As discussed in Section 4, the solution of non-convex MINLPs is not without it challenges. However, optimization of discrete variables with SM methods remains extremely challenging, as provable convergence to a local optimum is difficult to demonstrate.
- **Optimization decomposition methods:** EO modeling allows the use of powerful decomposition methods (Lagrangian, Schur complement, etc.) that break the original problem into more manageable subproblems. See Zhu et al. (2010, 2011) for examples of decomposition methods applied to very large scale process design problems under uncertainty.
- **Low cost sensitivity analysis:** Using EO methods, sensitivity information at the optimal solution is available as a byproduct of the solution procedure; KKT multipliers report the linearized sensitivity of the objective function with respect to perturbations in each bound and constraint. This information is especially valuable in process optimization studies, where one may be forced to rely on assumptions or weakly validated models that constrain the optimal value. In contrast performing sensitivity analysis around a solution with SM methods requires simulating the flowsheet at multiple design points around the optimal solution.

See Biegler et al. (1997) for further discussion of SM and EO flowsheeting methods.

Many opportunities exist for advancement of EO flowsheet methods, such as the development of robust initialization procedures, the refinement of optimization formulations to avoid integer variables and the application of decomposition methods for design under uncertainty. Tackling these challenges requires development of environments for EO flowsheet optimization that extend beyond existing commercial tools, both in terms of modeling flexibility and the ability to interface with numerous optimization algorithms. In this paper we present a new EO optimization framework and demonstrate its capabilities with a cryogenic air separation unit (ASU) synthesis study.

Two central themes are present throughout the framework: (1) refinement for robust initialization, and (2) modular equation-oriented models. Regarding initialization, the flowsheet is first optimized using simplified models for each core module. The simplified solutions are then used to initialize the more detailed (and difficult to optimize) models, resulting in an initialization procedure that has been quite successful with the ASU demonstration system. Regarding modularity, many of the units are generalized as thermodynamic equipment (requiring phase equilibrium calculations) or heat exchange equipment. These units inherit (borrowing a concept from computer science) equations from their generalized parent models, resulting in a concise framework that is easy to extend.

The remainder of the paper is organized as follows. First, the four core modules for the framework are introduced. In Section 2 the **thermodynamics module** is discussed. It contains both the ideal gas/correlation-based and the more rigorous cubic equation of state (CEOS) models. Results from optimization with the ideal gas model are used to initialize the CEOS variables. Strategies to accommodate vanishing phases for both models are examined. Next, in Section 3, the thermodynamic models are extended to a **common equipment model**. Refinements of the general model into specific types of units (flash vessels, throttle valves, etc) are discussed. In Section 4, two **models for distillation cascades** are presented. The first is an extension of the shortcut model developed by Kremser and refined by Edmister. The second is a new rigorous MESH model with tray bypass. Both of these approaches avoid integer variables, allowing the distillation models to be solved as a continuous nonlinear system. In Section 5, the Duran–Grossmann pinch based method for simultaneous **heat integration** and process optimization is discussed and modifications are presented. An approach to accommodate phase changes is incorporated, along with a model refinement technique to improve the constant heat capacity assumption. In Section 6 **practical concerns**, such as systematic initialization and avoiding degenerate equations are considered. The new EO framework is demonstrated in Section 7 in a **cryogenic air separation unit design case study** for advanced fossil fuel power plants. Finally, conclusions and future directions are discussed in Section 8.

2. Integrated thermodynamics models

For EO-based optimization, we begin with the underlying thermodynamic models that calculate properties (enthalpy, fugacity, etc.) used in each process stream. Two separate modules are included in the framework. The *simple* module relies on ideal gas assumptions and related correlations, and the second module uses *cubic equation of state* (CEOS) models (specifically Peng–Robinson or Soave–Redlich–Kwong) that are available in many common flowsheet simulators. The results from the simple module are used to initialize the CEOS equations.

The remainder of this section is organized as follows. First, we summarize vapor–liquid calculations with phase disappearance; this defines the strategy to model vanishing phases. Next both thermodynamics modules are introduced, along with a common stream model. Relaxation strategies are then applied to both modules to accommodate phase disappearance. Finally, an EO approach for phase verification is discussed.

2.1. Phase disappearance and VLE calculations

At the heart of optimization-based process synthesis is the concept of formulating a superstructure to simultaneously consider many different system configurations. Inevitably some streams in the superstructure will have no flow. For example, consider a flash vessel where each phase is modeled as a separate outlet stream in equilibrium. Both phases are present under only certain temperature, pressure and feed composition conditions (resulting in both outlet streams with positive flowrates). In all other cases, one of the streams will vanish and the constraints specifying phase and equilibrium relationships must be relaxed. In order to develop a robust VLE model, we start with the Gibbs free energy minimization problem and write the KKT optimality conditions (see Chapter 11 of Biegler (2010) for further details). After some reformulation of the fugacity formulas, the complementarity conditions are written as follows:

$$y_c = \beta K_c x_c \tag{1a}$$

$$-\sigma^L \leq \beta - 1 \tag{1b}$$

$$\beta - 1 \leq \sigma^V \tag{1c}$$

$$0 \leq L \perp \sigma^L \geq 0 \tag{1d}$$

$$0 \leq V \perp \sigma^V \geq 0 \tag{1e}$$

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