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Simultaneous process optimization and heat integration based on rigorous process simulations

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ABSTRACT

This paper introduces a simultaneous process optimization and heat integration approach, which can be used directly with the rigorous models in process simulators. In this approach, the overall process is optimized utilizing external derivative-free optimizers, which interact directly with the process simulation. The heat integration subproblem is formulated as an LP model and solved simultaneously during optimization of the flowsheet to update the minimum utility and heat exchanger area targets. A piecewise linear approximation for the composite curve is applied to obtain more accurate heat integration results. This paper describes the application of this simultaneous approach for three cases: a recycle process, a separation process and a power plant with carbon capture. Case study results indicate that this simultaneous approach is relatively easy to implement and achieves higher profit and lower operating cost and, in the case of the power plant example, higher net efficiency than the sequential approach.

1. Introduction

Heat integration plays a key role in improving energy efficiency and reducing operating costs in the energy and chemical industries. A number of methodologies have been developed in process systems engineering research for heat exchanger network synthesis (HENS). Linnhoff and Hindmarsh (1983) proposed the pinch design method, which is based on physical insight for the maximum heat recovery in heat exchanger networks. Papoulias and Grossmann (1983) and Cerda and Westerberg (1983) developed mathematical programming based methods for HENS. Detailed reviews of HENS methods are provided in several review articles: Gundersen and Naess (1988), Grossmann et al. (1999), Furman and Sahinidis (2002), Morar and Agachi (2010) and Klemeš and Kravanja (2013).

Two different approaches for combining heat integration and process optimization have been developed: sequential and simultaneous. Traditionally, a sequential strategy is applied when performing process optimization without heat integration, that is, the process is optimized in the first stage assuming all heating and cooling loads are provided by utilities; in the second stage, heat integration is performed after the optimal stream conditions (flow rates, temperatures, etc.) are identified (Biegler et al., 1997). Since heat integration is ignored during process optimization, the sequential approach may not fully optimize the whole process and may overestimate the utility cost. To overcome this drawback, Duran and Grossmann (1986) proposed a simultaneous strategy in which heat integration is performed in conjunction with process flowsheet optimization. In this strategy, a set of heat integration constraints that predict the minimum utility targets are added to the process optimization model. These constraints are based on a pinch location method so that heat integration can be performed under variable stream flowrates and temperatures. The authors also extended the pinch location method to cases with multiple utilities. A smooth approximation method was proposed to overcome non-differentiabilities in the optimization problem so that the entire problem can be solved as a regular NLP problem. The simultaneous strategy was demonstrated to achieve better economic performance, including both higher conversions of raw materials and lower total costs in recycle processes, compared to the sequential strategy (Duran and Grossmann, 1986; Lang et al., 1988). Grossmann et al. (1998) proposed an MINLP model for simultaneous process optimization and heat integration in which logic disjunctions were used to explicitly model the placement of streams for various potential pinch locations. This article also extended the application of the simultaneous strategy to cases with isothermal streams. Kamath et al. (2012) further extended the simultaneous strategy to cases with multistream heat

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exchangers (MHEX) and with process streams undergoing phase change; streams with phase change were split into substreams corresponding to each of phases, and a disjunctive representation was proposed to identify the phase for each substream. Papalexandri and Pistikopoulos (1998) developed a decomposition method for the solution of simultaneous process optimization and heat integration, where the heat integration problem was solved in an inner loop for a fixed process flowsheet and the process flowsheet was then optimized in an outer loop using the information from heat integration. Lang et al. (1988) implemented the simultaneous approach within the process simulator FLOWTRAN by adding the heat integration constraints developed by Duran and Grossmann (1986) to the process model in the simulator. The optimization was implemented using an SQP method, which assumes differentiability in the functions. Thus, newer derivative-free optimization solvers have not been used. In addition, this previous approach cannot handle cases where models of different units or subsystems are implemented in different process simulators.

The simultaneous optimization and heat integration approach has been applied to the optimal design of a wide range of processes, such as distillation systems (Novak et al., 1996), reaction/separation systems (Papalexandri and Pistikopoulos, 1998), hybrid thermochemical processes converting coal, biomass and natural gas to transportation fuel (CBGTL) (Baliban et al., 2011, 2012), biodiesel production processes (Martín and Grossmann, 2012), water networks (Yang and Grossmann, 2012; Kim et al., 2009), biorefinery processes (Ng et al., 2012; Wang et al., 2013; Gebreslassie et al., 2013), ethanol and food coproduction processes (Čuček et al., 2011), energy polygeneration processes (Chen et al., 2011a, 2011b), and offshore natural gas liquefaction processes (Wechsung et al., 2011). The simultaneous approach has also been used for the retrofit of chemical processes (Ponce-Ortega et al., 2008a).

However, the current simultaneous approach relies primarily on optimization models developed in equation-based modeling environments such as GAMS. Until recently, this capability has not been compatible with the more rigorous models implemented within the commercial flowsheet simulators that are widely used in power, chemical and oil industries, such as Aspen Plus, Aspen HYSYS, Aspen Custom Modeler (ACM), gPROMS and Thermoflex. Many simulation-based optimization technologies have been developed in recent years (Gosavi, 2003; Deng, 2007) and applied to the optimization of various processes utilizing rigorous simulator-based models, including pressure swing adsorption (PSA) processes (Rajasree and Moharir, 2000), power plants with carbon capture (Eslick and Miller, 2011), and supply chain networks (Wan et al., 2005; Mele et al., 2006). These advances in simulation-based optimization provide the foundation for the simultaneous optimization and heat integration approach proposed in this article.

This paper introduces a simultaneous process optimization and heat integration approach, which optimizes design parameters and operating conditions in the process flowsheet, using rigorous models in process simulators. Since the process models in simulators are usually large black box models that do not readily provide derivative information, this approach utilizes a derivative-free optimizer (DFO) (Conn et al., 2009; Kolda et al., 2003; Rios and Sahinidis, 2013) to optimize the overall process system. Links are established among the process simulators, the heat integration module and the DFO to realize efficient data transfer. For each iteration of the DFO, the process simulators converge the model for a set of design and operating conditions determined by the DFO. Stream temperatures and heating and cooling loads are exported to the heat integration submodel which is solved as a linear programming problem in GAMS for the minimum utility target and minimum heat exchanger area target. The results from both the process simulation and the heat integration submodel are then returned to the DFO and used to evaluate the overall objective function. Compared with the equation-based simultaneous approach, the proposed simulation-based simultaneous approach has several advantages. First, it treats simulations as black boxes and is easy to implement. Second, it does not require simplification of the process models. Hence, high-fidelity models can be used directly. Finally, it can be applied to processes in which unit models are developed in different process simulators. This paper describes the approach and demonstrates its capabilities on three industrial-scale cases: a methanol production process (with a recycle stream), a separation process for benzene, and a supercritical pulverized coal power plant with post-combustion carbon capture and compression.

The remainder of this paper is organized as follows. Section 2 introduces the overall simulation-based optimization approach with heat integration. Section 3 describes the heat integration module used in the simultaneous approach, including the LP models for the minimum utility target and the minimum heat exchanger area target. The piecewise linear approximation for the composite curve of streams is also described in Section 3. Finally, Section 4 discusses optimization and heat integration results for the three industrial-scale cases. The paper is concluded in Section 5.

2. Simultaneous process optimization and heat integration approach

2.1. Overview of the simultaneous approach

The simulation-based simultaneous optimization and heat integration approach is illustrated in Fig. 1 (Chen et al., 2014), where process simulators, the heat integration module and DFOs are tightly linked to each other. The DFO currently used in this approach is the Covariance Matrix Adaptation Evolutionary Strategy (CMA-ES) (Hansen, 2006), which is a global search optimization method suitable for difficult nonlinear nonconvex problems in continuous domains. Two process simulators, Aspen Plus and Aspen Custom Modeler (ACM) (AspenTech, 2014), have been utilized for simulation. Excel and Python are tightly integrated into the approach and are employed to perform cost evaluation and other post-simulation analysis. Support for additional process simulators, such as gPROMS Model Builder (PSE, 2014), is an active area of development. The heat integration module is developed in GAMS (McCarl et al., 2013), and it predicts the minimum utility target and minimum heat exchanger area target when provided with stream and equipment conditions.

The DFO is used to determine the values of the decision variables that maximize or minimize the value of an overall objective function. Within each iteration of the optimization algorithm the process simulation is converged and the heat integration problem is solved. First, the DFO selects an initial set of decision variables that are passed to the process simulators. The simulators converge the flowsheet using the values from the DFO. Relevant stream information (hot and cold stream flow rates, temperatures and enthalpies) and equipment information (heating or cooling loads and temperatures of equipment) are transferred from the simulators to the heat integration module. This module, which solves a linear programming problem, is then called to calculate the minimum utility cost (or consumption) and the minimum heat exchanger area while satisfying all heating and cooling loads. Using information from both the process simulations and the heat integration results, the overall system performance is evaluated in Python or Excel, to determine the value of the objective function and system constraints. Finally, the DFO determines new values for the decision variables. This procedure continues until the optimal solution is found or the maximum number of iterations is reached. Note that this approach is generally not well suited to optimization problems