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# A superstructure-based framework for simultaneous process synthesis, heat integration, and utility plant design

Lingxun Kong, S. Murat Sen, Carlos A. Henao, James A. Dumesic, Christos T. Maravelias*

*Department of Chemical and Biological Engineering, University of Wisconsin – Madison, Madison, WI 53706, USA*

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ABSTRACT

We propose a superstructure optimization framework for process synthesis with simultaneous heat integration and utility plant design. Processing units in the chemical plant can be modeled using rigorous unit models or surrogate models generated from experimental results or off-line calculations. The utility plant subsystem includes multiple steam types with variable temperature and pressure. For the heat integration subsystem, we consider variable heat loads of process streams as well as variable intervals for the utilities. To enhance the solution of the resulting mixed-integer nonlinear programming models, we develop (1) new methods for the calculation of steam properties, (2) algorithms for variable bound calculation, and (3) systematic methods for the generation of redundant constraints. The applicability of our framework is illustrated through a biofuel case study which includes a novel non-enzymatic hydrolysis technology and new separation technologies, both of which are modeled based on experimental results.

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## 1. Introduction

A superstructure refers to a process diagram that includes all potentially useful processing units and all relevant connections. Superstructure frameworks have been proposed for solving process synthesis problems (Barnicki and Siirola, 2004; Siirola, 1995; Trespalacios and Grossmann, 2014; Yeomans and Grossmann, 1999). By solving the superstructure optimization model, all process alternatives embedded are evaluated, and the best alternative is selected along with the optimal operation conditions for each unit.

Superstructure-based approaches have the advantage of simultaneously considering complex interactions between all design decisions. To identify good designs however the development of a rich superstructure is necessary, and at the same time rigorous unit operation models have to be used to obtain accurate results. Therefore, the resulting formulations are large-scale non-convex mixed-integer nonlinear programming (MINLP) models (Fig. 1).

In terms of superstructure generation, early works focused on the combination of simple structures formulated based on engineering judgment (Kocis and Grossmann, 1989) and the combination of superstructure subsystems (e.g. reaction network, separation network, and heat recovery network) each created independently (Achenie and Biegler, 1990; Floudas et al., 1986; Floudas and Paules, 1988; Hasan et al., 2010; Kokossis and Floudas, 1994; Lakshmanan and Biegler, 1996; Novak et al., 1996; Ponce-Ortega et al., 2008; Schweiger and Floudas, 1999; Yee and Grossmann, 1990). Friedler et al. later proposed a mathematical framework for the creation of superstructures and an algorithm to generate the so-call "maximal structure" (Friedler et al., 1992).

Once the superstructure is generated, all the units must be accurately modeled. In many cases, to ensure that the resulting superstructure model is computationally tractable, rigorous unit models are replaced by approximate models (e.g. shortcut methods). Aggarwal and Floudas proposed linear and bilinear approximations for the component split fractions in modeling separators (Aggarwal and Floudas, 1990); Bausa et al. incorporated the classic Underwood methods with other proposed techniques and developed a more general shortcut method called rectification body method (RBM), which is applicable to non-ideal multicomponent distillation with arbitrary splits (Bausa et al., 1998); Yeomans and Grossman applied first principles models with simplified kinetics and thermodynamic properties to model tray-by-tray ideal distillation models (Yeomans and Grossmann, 2000); Kraemer et al. developed a shortcut-based design method for multicomponent heteroazeotropic distillation (Kraemer et al., 2011); Bruggemann and Marquardt proposed an optimization-based conceptual design framework for finding the optimal recycle policy for azeotropic distillation (Bruggemann and Marquardt, 2011). However, the aforementioned methods address subsystems of a process.

* Corresponding author. Tel.: +1 6082659026; fax: +1 6082625434.

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**Notation**

*Sets*

| | |
|---|---|
| $i \in \mathbf{I}$ | units |
| $j \in \mathbf{J}$ | process streams |
| $k \in \mathbf{K}$ | components |
| $m \in \mathbf{M}$ | temperature intervals |
| $n \in \mathbf{N}$ | number of stages in multi-stage extraction units |
| $r \in \mathbf{R}$ | reactions |
| $u \in \mathbf{U}$ | utilities for cooling/heating |

*Subsets*

| | |
|---|---|
| $\mathbf{J^C}/\mathbf{J^H}$ | cold/hot process streams |
| $\mathbf{J^{UN}}/\mathbf{J^{US}}$ | cold/hot utility streams |
| $\mathbf{J}_i$ | streams connected to unit $i$ |
| $\mathbf{J}_i^{\mathrm{IN}}/\mathbf{J}_i^{\mathrm{OUT}}$ | inlet/outlet streams of unit $i$ |
| $\mathbf{M}_j$ | temperature intervals that stream $j$ spans |
| $\mathbf{U^S}$ | utilities for heating |
| $\mathbf{U^N}$ | utilities for cooling |

*Parameters*

| | |
|---|---|
| $\Delta S^{cond}$ | entropy of condensation of steam (kJ/kg K) |
| $\Delta T^{min}$ | minimum temperature difference for heat exchange (K) |
| $\eta_i$ | efficiency of unit $i$ |
| $\kappa_{i,n}^k$ | recovery of component $k$ if $n$ stages are selected for multi-stage extraction unit $i$ |
| $\xi_{i,k}$ | partition coefficient of component $k$ in extraction unit $i$ |
| $Cp_j$ | specific heat capacity of process stream $j$ (kJ/kg K) |
| $LHV_k$ | lower heating value of component $k$ (kJ/kg) |
| $R^{univ}$ | universal gas constant (kJ/kmol K) |

*Continuous variables*

| | |
|---|---|
| $\gamma_{u,u'}$ | expansion coefficient of turbine (inlet steam $u$ and outlet steam $u'$) |
| $\delta_{u,u'}^+, \delta_{u,u'}^-$ | deviation variables for isentropic expansion |
| $\varepsilon_{u,u'}^+, \varepsilon_{u,u'}^-$ | deviation variables for isenthalpic expansion |
| $\psi_i$ | unit internal variables for unit $i$ |
| $\Omega_{i,k}$ | component recovery of $k$ in separation unit $i$ |
| $C_r$ | conversion of the limiting component in reaction $r$ |
| $Cc$ | total annualized capital cost (MM$/yr) |
| $F_{j,k}$ | molar flow rate of component $k$ in stream $j$ (kmol/h) |
| $F_j^T$ | total molar flow rate of stream $j$ (kmol/h) |
| $H_j$ | enthalpy of stream $j$ (kJ/kg) |
| $Co$ | operating cost (MM$/yr) |
| $P_j$ | pressure of stream $j$ (bar) |
| $P_j^{red}$ | reduced pressure of stream $j$ |
| $Q^{cond}$ | cooling required for condensation of the wet steam (kW) |
| $Q_i$ | heat load for unit $i$ (kW) |
| $Q_j^h$ | heat available in hot utility stream $j$ (kW) |
| $Q_{j,m}^h/Q_{j,m}^c$ | heat provided/received by hot/cold stream $j$ in interval $m$ (kW) |
| $QR_m$ | residual heat from interval $m$ to interval $m+1$ (kW) |
| $T_j$ | temperature of stream $j$ (K) |
| $T_j^{red}$ | reduced temperature of stream $j$ |
| $T_{j,m}^h$ | temperature of hot utility stream $j$ in interval $m$ (K) |
| $T_u^{sat}$ | saturation temperature of steam $u$ (K) |
| $W^{demand}$ | electricity demand (kW) |
| $W^{purchase}$ | amount of electricity purchased (kW) |
| $W^{sale}$ | excess electricity sales (kW) |
| $W_i$ | power requirement of unit $i$ (kW) |
| $X_{j,k}$ | mole fraction of component $k$ in stream $j$ |
| $Z_u$ | compressibility factor of steam $u$ |

*Binary variables*

| | |
|---|---|
| $Y_i^{unit}$ | 1 if unit $i$ is selected |
| $Y_{i,n}^{mse}$ | 1 if there are $n$ stages in the multi-stage extraction unit $i$ |
| $Y_{j,m}$ | 1 if temperature of steam $j$ is in interval $m$ |

Ideally, when solving process synthesis problems, we would like to integrate the design of the chemical plant with the design of the utility system and the heat recovery network. Papoulias and Grossman proposed a mixed-integer linear programming (MILP) formulation that integrates the three subsystems (Papoulias and Grossmann, 1983b). Colmenares and Seider used a non-linear programming (NLP) model for integrating the design of the chemical plant with the utility plant (Colmenares and Seider, 1989). More rigorous MINLP models were proposed later, including more accurate models for steam and gas turbines (Mavromatis and Kokossis, 1998; Varbanov et al., 2004; Wilkendorf et al., 1998); accurate steam property estimation (Aguilar et al., 2007; Bruno et al., 1998; Caballero et al., 2014; Rodriguez-Toral et al., 2001); and operational planning of utility systems (Francisco and Matos, 2004; Iyer and Grossmann, 1998). One limitation of the previous studies is the assumption that heating utilities have constant temperatures and pressures. A more realistic approach would be to allow steam temperatures and pressures to vary continuously and then accurately calculate steam thermodynamic properties (e.g. enthalpy) as a function of steam temperatures and pressures.

To address these challenges, we propose a superstructure framework that allows us to simultaneously perform (1) structural and parametric optimization for the chemical plant, (2) heat integration, and (3) utility plant design. To obtain realistic yet computationally tractable optimization models, we (1) employ unit surrogate models generated from experimental results or off-line simulations using rigorous models, (2) develop new expressions for the calculation of steam thermodynamic properties, (3) develop algorithms for the calculation of tight variable bounds, and (4) develop systematic ways for the generation of redundant constraints.

The paper is structured as follows. In Section 2, we present the superstructure modeling framework consisting of three main subsystems: the chemical plant, the heat integration subsystem, and the utility plant along with a thermodynamic properties calculation module. In Section 3, we discuss the algorithms for the calculation of variable bounds and the generation of redundant constraints. Finally, in Section 4, we illustrate the applicability of the proposed framework through the design of a lignocellulosic ethanol facility employing a novel non-enzymatic biomass hydrolysis technology.

## 2. Superstructure modeling framework

The conceptual integration of the chemical plant, heat integration, and utility plant subsystems is illustrated in Fig. 2. We develop general modeling strategies for each subsystem, and identify the variables that connect them. While all subsystems are connected with each other, the modeling equations for each one of them are independent from each other; they are interfaced via some interconnecting variables (to be discussed later). Thus, the integrated

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