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Modeling phase changes in multistream heat exchangers

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ABSTRACT

A new method for modeling phase changes in multistream heat exchangers (MHEXs) is presented. In many industrially relevant applications, streams in MHEXs will undergo phase changes between their inlet and outlet. In this model, nonsmooth equations are formulated which properly account for the existence or nonexistence of phases in heat integration, flash and physical property calculations in a MHEX. These new equations are used in conjunction with a recently developed nonsmooth model for MHEXs to create a compact equation system which can be used for the simulation and design of complex processes. Notably, this formulation does not involve the solution of a difficult optimization problem, since it avoids the use of either disjunctive or complementarity constraints. The robustness and functionality of the new formulation is illustrated through several simulations of the well-known Poly Refrigerant Integrated Cycle Operations (PRICO) process for liquefied natural gas production.

1. Introduction

Multistream heat exchangers (MHEXs) are commonly found at the heart of many industrially relevant cryogenic processes, such as natural gas liquefaction processes. However, among the many difficulties of simulating MHEXs in cryogenic processes is the detection and handling of phase changes. Taking liquefied natural gas (LNG) production as an example, the streams in the process MHEXs are usually both multicomponent and multiphase. Handling the nonlinear physical property variations associated with such streams during heat exchange creates a challenging simulation problem, especially when the phases traversed are not known *a priori*.

Methods for multiphase MHEX or heat exchanger network simulation have been reported by several authors in the literature. Among these, the focus is often placed on modeling pure component (isothermal) phase changes. An early approach along this theme is that of Grossmann et al. [1], which adapts the earlier Duran and Grossmann [2] model for simultaneous process optimization and heat integration by accounting explicitly for streams which are known to be isothermal. This is done with the use of disjunctive constraints, which are reformulated with binary variables to yield a mixed-integer nonlinear program (MINLP). Ponce-Ortega et al. [3] tackle isothermal streams in the context of heat exchanger network synthesis by applying a similar extension to the classic staged-superstructure approach from Yee and Grossmann [4]. However, these methods for isothermal phase changes do not extend to methods for the multicomponent case, which are more relevant for many practical applications.

Several approaches do exist in the literature for handling non-isothermal phase changes. Castier and Queiroz [5] describe a method based on solving a series of global optimization problems in successive temperature intervals to find pinch points and minimum energy targets in a HEN where the temperature-enthalpy relationship is possibly nonlinear. While more precise than methods that use piecewise-affine segments to approximate the composite curves, the approach requires significant computational effort.

Hasan et al. [6,7] use the superstructure concept as a basis for their work with mixed refrigerant processes by deriving a network of two-stream heat exchangers which is equivalent to an MHEX. This model handles phase changes in an MHEX by modeling the heat transfer in each phase as taking place in a separate two-stream heat exchanger in the superstructure bundle. The existence of the heat exchangers is determined by a disjunctive formulation and a set of propositional logic constraints to formulate a very complex MINLP. The bubble and dew points are taken as constants in their model, so that stream pressures and compositions cannot change during optimization. Additionally, the temperature-enthalpy relationship in each phase is given by an empirical cubic correlation instead of a rigorous physical property model.

An alternate method for modeling phases changes in MHEX which is also based on the Duran and Grossmann [2] formulation is given by Kamath et al. [8]. Here, the authors make the analogy between a heat exchanger network which requires no external

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Nomenclature

A	heat transfer area (m^2)
C	index set of cold streams
EBP	extended pinch location function (W)
F	molar flowrate ($mol \cdot s^{-1}$)
F_{C_p}	heat capacity flow rate of hot stream ($W \cdot K^{-1}$)
f_{C_p}	heat capacity flow rate of cold stream ($W \cdot K^{-1}$)
$\mathbf{G}$	element of generalized derivative
H	index set of hot streams
K	equilibrium coefficient
L	liquid phase molar flowrate ($mol \cdot s^{-1}$)
n	total number
P	index set of pinch candidates
$\mathcal{PC}^1$	class of piecewise-differentiable functions
Q	heat flowrate (W)
h	specific enthalpy ($J \cdot mol^{-1}$)
s	slack variables in flash complementarity formulation
T	temperature of hot stream (K)
t	temperature of cold stream (K)
$\mathbf{u}$	unknown variables
U	overall heat transfer coefficient ($W \cdot m^{-2} \cdot K^{-1}$)
V	vapor phase molar flowrate ($mol \cdot s^{-1}$)
$\mathbf{x}$	liquid phase mole fraction vector
X	set of bounds on the variables $\mathbf{u}$
$\mathbf{y}$	vapor phase mole fraction vector
Y	indicator variable in disjunctive formulation
$\mathbf{z}$	feed stream mole fraction vector

Greek symbols

β	variable used to relax equilibrium constraints
γ	variable in LP objective of the LP-Newton method
ΔT_{LM}	log-mean temperature difference (K)
ΔT_{min}	minimum approach temperature between hot and cold streams (K)
ε	user-defined parameter for streams with small temperature change (K)

Subscripts

2p	two-phase region
BP	bubble point
DP	dew point
F	feed
i, j	stream or component indices
L	liquid phase
sub	subcooled phase region
sup	superheated phase region
V	vapor phase

Superscripts

c	critical
d	nondifferentiable point or endpoint
k	iteration counter
IN/OUT	inlet/outlet of physical process stream
in/out	inlet/outlet of heat integration stream

utilities and an MHEX to derive an equation-oriented model. The authors use a simpler disjunctive representation of the phase detection problem than Hasan et al. [7], which is subsequently handled by using complementarity constraints rather than binary variables. The model is also able to incorporate thermodynamics described by cubic equations of state. Applied to the Poly Refrigerant Integrated Cycle Operations (PRICO) process, the formulation results in a moderately-sized mathematical program with complementarity constraints (MPCC) (3426 equations using Soave-Redlich-Kwong thermodynamics) which requires completing a rather involved initialization procedure to obtain a suitable initial guess from which to solve the problem and a solution method suitable for MPCCs.

Of particular note here is that all the approaches mentioned above require the solution of a hard optimization problem, with those methodologies which involve the solution of a nonconvex MINLP being particularly challenging. Among the approaches which avoid the use of binary variables, the use of smoothing approximations to remove the nonsmoothness caused by approximating the temperature-enthalpy relationship of streams as a piecewise-affine function is common. This is often done with the reformulation of the max operator presented by Balakrishna and Biegler [9]. In contrast, the model presented in this work is presented as an equation solving problem, rather than an optimization problem. Furthermore, the equations developed herein are substantially simpler than the mixed-integer or complementarity constraint formulations developed in previous works, at the expense of being nonsmooth. However, this is no longer a significant obstacle to practical implementation due to the recent development of automatic techniques to calculate generalized derivatives [10] and robust methods for nonsmooth equation solving [11,12]. The model size and problem complexity is thereby substantially reduced compared to the models presented thus far in the literature.

2. Background

2.1. A nonsmooth model for MHEX simulation

Consider the multistream heat exchanger model shown in Fig. 1, in which a set of hot streams, indexed by a set H, exchange heat with a set of cold streams, indexed by a set C. Each hot stream $i \in H$ enters at temperature T_i^{in}, exits at temperature T_i^{out} (with $T_i^{in} \geqslant T_i^{out}$) and has a constant molar heat capacity flowrate $F_{C_p,i}$, which is defined as the product of the molar flowrate F_i and the (assumed constant) molar heat capacity $C_{p,i}$ of the stream at representative conditions. Similarly, each cold stream $j \in C$ enters at temperature t_j^{in}, exits at temperature t_j^{out} (with $t_j^{in} \leqslant t_j^{out}$) and has a constant molar heat capacity flowrate $f_{C_p,j}$.

As shown in the figure, the specific model under consideration is a countercurrent exchanger, wherein all hot streams are

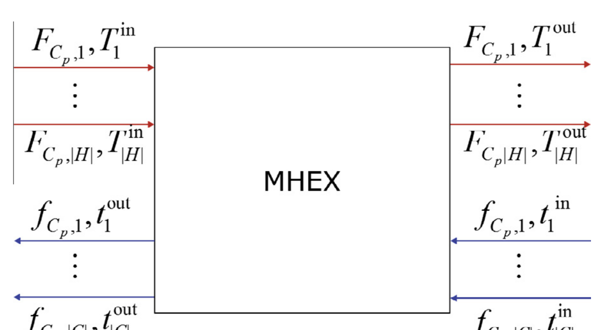

Fig. 1. Schematic of a multistream heat exchanger with $|H|$ hot streams and $|C|$ cold streams.