Combined simulation–optimization methodology for the design of environmental conscious absorption systems

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ABSTRACT

This work addresses the optimization of ammonia–water absorption cycles for cooling and refrigeration applications with economic and environmental concerns. Our approach combines the capabilities of process simulation, multi-objective optimization (MOO), cost analysis and life cycle assessment (LCA). The optimization task is posed in mathematical terms as a multi-objective mixed-integer nonlinear program (moMINLP) that seeks to minimize the total annualized cost and environmental impact of the cycle. This moMINLP is solved by an outer-approximation strategy that iterates between primal nonlinear programming (NLP) subproblems with fixed binaries and a tailored mixed-integer linear programming (MILP) model. The capabilities of our approach are illustrated through its application to an ammonia–water absorption cycle used in cooling and refrigeration applications.

1. Introduction

The worldwide cooling demand has drastically increased over the last few years, which has led to the installation of a large number of air conditioning systems (Balaras et al., 2007; Henning, 2007). This has resulted in a dramatic rise in electricity consumption, which is nowadays mostly generated from fossil fuels. This trend has caused important environmental problems such as ozone layer depletion and global warming. In this general context, there is a clear need to develop environmentally friendly and energy efficient technologies in order to minimize the environmental impact of cooling applications. Particularly, absorption systems have emerged as a promising alternative to conventional compression cycles (Florides, Kalogirou, Tassou, & Wrobel, 2002; Herold,

Radermacher, & Klein, 1996; McMullan, 2002), since they can use low grade energy sources that are environmentally friendlier.

Absorption machines use a mixture of a refrigerant and an absorbent. The most widely employed mixtures are ammonia–water (ammonia as refrigerant) and water–lithium bromide (water as refrigerant). An important difference between absorption and compression refrigeration systems lies in the energy source. Compression systems require electrical energy for its operation, whereas absorption systems can use low grade heat sources as energy input. Thus solar energy or waste heat (Keil, Plura, Radspieler, & Schweigler, 2008), can be used for saving up to 50% of the primary energy required for the provision of useful heat (Ziegler, Kahn, Summerer, & Alefeld, 1993). Energy conservation via waste heat recovery has been the focus of an increasing interest in the literature (Erickson, Anand, & Kyung, 2004). These systems can reduce global warming emissions (Darwish, Al-Hashimi, & Al-Mansoori, 2008) and mitigate as well the ozone layer depletion. They show a high reliability and a silent and vibration free operation. Unfortunately, absorption cycles require more units than compression cycles, which leads to larger capital investments.

Finding ways to improve the efficiency of absorption systems has recently attracted an increasing interest (Darwish et al., 2008). In order to promote the use of absorption systems and to ensure their competitiveness with respect to conventional compression systems, it is still necessary to further improve their performance and reduce their cost. This can be accomplished by developing

Nomenclature

Sets/indices

B	environmental burdens indexed by b (i.e., feedstock requirements, emissions and waste)
D	decision variables indexed by d
i	topology
j	external equality and inequality constraints
$j \in EQ$	external (explicit) equality constraint
$j \in IEQ$	external (explicit) inequality constraint
k	iteration
M	equipment units indexed by m
$m \in HX$	heat exchangers
o	objective functions

Variables

A_m	area of heat exchanger m (m^2)
C_{HX}	cost of heat exchangers (€)
C_P	cost of the pumps (€)
C_{RC}	cost of the rectification column (€)
CF	annual capital cost (€)
Cb	exchange area (m^2)
C_m	cost of unit m (€)
CO	operating cost (€/year)
DAM_d	environmental damage in category d (points)
$Diam$	diameter of the rectification column (m)
$df_{b,d}$	damage in category d per unit of b (points/kg)
EI	environmental impact (points)
H	height of the rectification column (m)
LCI_b	life cycle inventory entry associated with b (kg)
Q_m	heat transfer of unit m (kW)
W_m	mechanical power of unit m (kW)
ΔT_m^{lm}	logarithmic mean temperature difference of unit m (K)
α	auxiliary variable
$\prod$	penalty value for constraint violation

Parameters

c_1	cost parameter (€/m^2)
c_2	cost parameter (€)
c_3	cost parameter (€/kW)
cq	unitary cost of steam (€/MJ)
cw	unitary cost of electricity (€/MW h)
crf	capital recovery factor
Fc	cost factor that depends on the type of column
fd	design coefficient
fp	design coefficient
fm	material construction coefficient
$M\&S$	Marshal & Swift equipment cost index
n	number of objective functions
top	operational hours (h/year)
U_m	overall heat transfer coefficient of unit m (kW/m^{2}K)
χ_{euro}	conversion from dollars to euros (€/$)

systematic strategies to assist in their design. Thermoeconomic optimization is well suited to address this problem, since it allows performing energy and economic analysis for different configurations and operating conditions in a systematic and rigorous manner (Kizilkan, Sencan, & Kalogirou, 2007; Misra, Sahoo, & Gupta, 2005, 2006; Selbas, Kizilkan, & Sencan, 2006).

Particularly, methods based on mathematical programming have recently gained wider interest in the optimization of cooling systems. Most of these approaches have focused on optimizing the economic performance of ammonia–water absorption

refrigeration systems (AWRS). One of the first optimization models for absorption cycles was the one introduced by Fernandez-Seara, Sieres, and Vazquez (2003). More recently, Chavez-Islas and Heard (2009a) and Chavez-Islas and Heard (2009b) presented an equation-oriented method and a mixed-integer nonlinear programming (MINLP) model for the economical optimization of these systems. The same authors introduced an MINLP that considers different types of heat exchangers (Chavez-Islas, Heard, & Grossmann, 2009). Gebreslassie, Guillén-Gosálbez, Jiménez, and Boer (2009a) addressed also the optimization of a simplified AWRS considering uncertainties in the economic parameters.

These works focused on optimizing the economic performance as unique criterion. New trends have motivated the development of systematic strategies for optimizing the environmental impact of thermodynamic cycles along with their economic performance. Particularly, a promising strategy to accomplish this task relies on combining multi-objective optimization (MOO) tools with economic analysis and life cycle assessment (LCA) principles. This approach allows automating the search for alternatives leading to life cycle environmental savings (see Azapagic & Clift, 1999a). The overwhelming majority of this type of strategies that provide decision-support for environmentally conscious process designs have focused on the chemical sector. In contrast, these techniques have not been used to the same extent in energy applications. Some examples on the combined use of LCA and MOO can be found in the works by Azapagic and Clift (1999b) (production of boron compounds), Alexander, Barton, Petrie, and Romagnoli (2000) (design of a nitric acid plant), Carvalho, Gani, and Matos (2006) (design of a methyl tertiary butyl ether plant) and Guillen-Gosalbez, Caballero, and Jiménez (2008) (optimization of the hydrodealkylation of toluene), among some others.

Hence, the optimization of energy systems, and in particular, of cooling and refrigeration cycles with environmental concerns has received little attention to date. To the best our knowledge, Gebreslassie, Guillén-Gosálbez, Jiménez, and Boer (2009b) were the first to address the multi-objective optimization of absorption cycles with economic and environmental concerns. The main limitation of this work is that it relies on "short-cut" models of the process units, that is, on simplified equations that avoid the numerical difficulties associated with the nonlinearities and nonconvexities of the detailed equations of the process units of the cycle. These simplified models work well within a given range of operating conditions, but may perform poorly outside these intervals. Particularly, the generator of the cycle is a key unit that requires the use of complex thermodynamic packages for predicting the liquid–vapor equilibrium and stream properties (e.g., enthalpies, vapor pressures, etc.). Attempting to model this unit by short-cut formulations may lead to poor predictions, especially when working under refrigeration conditions.

This work introduces a systematic tool for the optimal design of absorption systems that aims to overcome the limitations mentioned above. Our approach is based on the combined use of process simulation and optimization tools (Brunet, Guillen-Gosalbez, Pérez-Correa, Caballero, & Jimenez, 2012; Caballero, Milán-Yañez, & Grossmann, 2005; Diaz & Bandoni, 1996; Diwekar, Grossmann, & Rubin, 1992; Kim, Kim, & Yoon, 2010; Kravanja & Grossmann, 1996; Reneaume, Koehret, & Joulia, 1995). One of the main advantages of our strategy is the use of detailed process models of the cycle, including a rigorous tray-by-tray formulation of the rectification column, all of which are implemented in a commercial process simulator (i.e., Aspen Plus). This avoids the definition of the underlying equations of the process units in an explicit form, taking advantage of the customized unit operations models and tailored solution algorithms already implemented in the process simulator. Furthermore, our method improves the robustness and numerical performance of the optimization algorithm, which is likely to