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# Optimization Framework for Energy-Induced Separation Network: Application to the Chilling Train System in Ethylene Plants

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The mass-exchange equilibrium relation depends on the temperature and pressure. Therefore, there are strong interactions between heat-exchange network and mass-exchange network. A modular framework methodology that combines the commercial sequential process simulator and optimization tools is proposed to perform the energy-induced separation network synthesis. As a case, the synthesis of the chilling train process in ethylene plants is used to illustrate the applicability of the proposed approach.

# 1. Introduction

The EISEN synthesis with simultaneous heat, mass and power exchange is the extension of heat-induced separation network (HISEN), which was originally developed for the separation systems that employ energy separating agents. EISEN refers to a network of heat exchangers and also pressure-adjusting devices that realizes a separation target via latent heat exchange. Dunn and EI-Halwagi (1994) presented the HISEN synthesis for single component and multicomponent volatile organic compounds (VOC) systems involved a three-stage targeting approach. EI-Halwagi et al. (1995) first proposed the essence of HISEN synthesis and developed a systematic two stage procedure to synthesize HISENs. Richburg and EI-Halwagi (1995) introduced a graphical approach to the optimal design of heat-induced separation networks for VOC recovery. Dunn and Dobson (1998) proposed a spreadsheet based approach to identify cost-effective heat-induced and energy-induced separation networks for condensation-hybrid processes. Although these methods have also proved their usefulness for in-plant waste minimization and source reduction, they are limited to ad hoc applications by their solo-dimensionality (Sharifzadeh et al., 2010). Therefore, these methods can not deal with the cases that require complex liquid phase mass integration or shaft power integration.

Recently, Hamad and Fayed (2004) employed process simulators to capture the non-ideality of the mixture equilibrium in order to construct the temperature path of the condensing fluid. Sharifzadeh et al. (2010) presented a simulation-optimization framework method that simultaneously consider all the conflicting tasks of mass, heat, and power exchange. Generally, the methodologies in previous work on the synthesis only deal with an economic objective function that guarantees the optimality of the design solution. However, in EISEN systems, there are often two conflicting objectives (separation degree and energy consumption). These two objectives conflict with one another-improvement in one objective is accompanied by deterioration in another objective, and so there will not be a single optimum.

In this paper, we develop a modular framework methodology that combines the commercial sequential process simulator and optimization tools to perform the EISEN synthesis for a chilling train process in ethylene plants. Single objective (minimize energy consumption only, minimize ethylene loss only, or maximize hydrogen recovery rate only) and multi-objective process synthesis models (two objective process synthesis and triple objective process synthesis) are discussed using the proposed methodology, respectively.

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#### 2. The General Optimization Framework for the Energy Induced Separation Network

Given a set of rich (waste) gaseous streams, a set of energy separating agents (ESA), synthesize a network of indirect-contact heat-induced separators along with pressurization/depressurization devices, which can recover a certain fraction of condensable species at specific objectives. The general EISEN problem representation figure can be found in the literature (Dunn and EI-Halwagi, 2003).

In this paper, the proposed modular integrated framework (Wang et al., 2013) that combines the commercial sequential process simulator and optimization tools is employed to perform the EISEN synthesis. To define process synthesis master task in the modular framework methodology, we firstly identify and classify the different types of variables that arise in an optimization problem in the modular framework methodology.

(1) Design variables or independent variables  $(x_i)$ .

In a chemical process simulator, these variables are the basic input conditions to converge the flowsheet. The number of such variables depends on the degrees of freedom in the flowsheet. Note that  $x_i$  includes both continuous variables (pressures, temperatures, flow rates, etc.) and discrete variables (i.e. number of stages, feed tray location).

(2) Variables calculated by the simulator (xc)

These are variables calculated by the simulator. Usually, the user can access these variables in read-only mode and has no direct control over these variables.

(3) Constraint variables  $(x_e)$ .

These variables represent the variables that do not appear at the flowsheet level but appear in explicit external constraints in the process synthesis level. Theses variables include the equality constraint variables h and inequality constraint variables g.

(4) Synthesis variables (y).

The synthesis variables are a set of binary variables that denote the potential existence (i.e.,  $y_i = 0$ ) or not (i.e.,  $y_i = 0$ ) of a process unit or techniques i in the optimal process. The synthesis variables determine the topology of the process (i.e., the selection of the applicable separation technique, selection of the separating agents).

Based on the variables mentioned above, if only one objective was considered in process synthesis, the mathematical model of the synthesis master task can be formulated as a MINLP problem with the following form:

$$\min_{x_{1}, x_{C}, y} f(x_{I}, x_{C}, y)$$
  
s.t.  
$$h(x_{I}, x_{C}, y) = 0$$
  
$$g(x_{I}, x_{C}, y) \le 0$$
  
$$x_{I} \in X_{I}^{m}$$
  
$$x_{C} \in X_{C}^{n}$$
  
$$y \in Y = \{0, 1\}^{l}$$

(1)

## 3. Case Study: Design and operation of the chilling train system

The chilling train system is an important part for ethylene plants, where the charge gas from the upper stream process is refrigerated to a very low temperature (lower than -160 °C) to separate hydrogen and methane and the left charge gas is sent to the Demethanizer Tower. Its design and operation significantly influence energy consumption and product loss rates (Zhang et al., 2010). On the basis of chilling train system analysis, the compressor can be placed in four locations before the first four flash drums as shown in Figure 1. The alternative positions generate the superstructure for a chilling train system design. Table 1 gives feed conditions of the charge gas.

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Table 1 Feed conditions of the charge gas

	Flowrate	ate Temperature Pressure		Composition (mol%)					
(	(kmol/h)	(°C)	(MPa)	H <sub>2</sub>	$CH_4$	$C_2H_4$	$C_2H_6$	$C_3H_6$	$C_3H_8$
Charge gas	8,000	-19.6	1.75	13.95	23.83	43.43	5.96	10.62	2.21



Figure 1 Compressor alternative position for chilling train system. CPHX, HX1, HX2, HX3, HX4, HX5, HX6, HX7, HX8: heat exchanger; CP1: Compressor; FLS1, FLS2, FLS3, FLS4: flash drums; VV1, VV2: throttling valve

The chilling train system involves three objectives: to minimize total energy consumption( $J_1$ ), to minimize ethylene loss ( $J_2$ ), and to maximize hydrogen recovery amounts ( $J_3$ ). The multi-objective optimization problem is formulated as

$\min J_1 = \sum_{u \in HX} E_u + \sum_{u \in CP} W_u$	(2)
min $J_2 = F_{S_8} M_{C_2 H_4, S_8}$	(3)
min $J_3 = F_{S_{H_2}} M_{H_2, S_{H_2}}$	(4)

Subject to

$-77 \le T_{FLS1} \le -67$	(5)
FLST	(-)

$-110 \le T_{FLS2} \le -100$	(6)
120 < T < 120	(7)

$$-130 \le T_{FLS1} \le -120 \tag{7}$$

$$-140 \le T_{FLS1} \le -135 \tag{8}$$

$$-165 \le T_{FLS1} \le -160$$
 (9)

$$3.2 \le P_{CP1} \le 3.6$$
 (10)

$$y_A + y_B + y_C + y_D = 1$$
(11)

$$y_A, y_B, y_C, y_D \in (0, 1)$$

In the energy objective function, the total energy consumption is characterized by the summation of exergy consumption from all the heat exchangers and work consumption (W) from all the compressors. Because the hydrogen product can be used as hydrogen source for other facilities, the hydrogen purity specification is regarded as a constraint.

When single objective process synthesis is considered, the task is to determine the optimal location of compressor and the optimal operational conditions for process units. The resulted based on Evol algorithm are summarized in table 2.

Conditions	Minimize energy consumption only	Minimize ethylene loss only	Maximize hydrogen recovery rate only
Temperature of FLS1 (°C)	-67.09	-76.97	-67.07
Temperature of FLS2 (°C)	-100.02	-109.94	-100.67
Temperature of FLS3 (°C)	-120.01	-130.00	-129.99
Temperature of FLS4 (°C)	-136.25	-136.98	-135.11
Temperature of FLS5 (°C)	-161.09	-164.90	-161.91
Discharge pressure of CB1 (MPa)	3.2009	3.5942	3.2011
Total energy (kW)	23,535	27,009	24,423
Hydrogen recovery rate (kmol/h)	1,061.9	1,052.5	1,067.0
Ethylene loss rate (kmol/h)	33.2	2.5	9.4
Compressor work (kW)	1,502	2,220	1,301
Hydrogen purity (mol%)	0.9667	0.9623	0.9501
Position of compressor	Position D	Position B	Position D

Table 2: Results based or	n Evol algorithm fo	or single objective	process synthesis
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As shown in Table 2, when minimizing the energy consumption only, the compressor is located in position D and ethylene loss rate reaches at 33.2 kmol/h. The temperatures of the flash drums tend to upper boundary while discharge pressure of the compressor tend to lower boundary, which cause less ethylene to be liquefied and lost in the vapor phase. On the contrary, when the temperatures of the flash drums tend to lower boundary while discharge pressure of the compressor tend to upper boundary, the objective of minimize ethylene loss rate can be obtained in Position B. It can also be seen that when the operation temperature of the flash drums tend to upper boundary, more hydrogen will be stay in vapor stream. Thus the hydrogen recovery rate can be maximized in Position D.



Figure 2 Pareto set of the simultaneous minimization for ethylene loss rate and energy consumption

As the optimal set is generated with respect to different objectives, the Pareto frontier is the optimal tradeoff between the objectives. Figure 2 shows the numeric results of the simultaneous minimization for ethylene loss rate and energy consumption. In the Pareto frontier, with the increase of energy consumption, the ethylene loss rate is reduced. The choice of the location for the compressor depends on the trade off between energy consumption and ethylene loss rate, i.e. Position B for lower energy consumption 23.94 MW with ethylene loss rate 25.6 kmol/h, and position D for lower ethylene loss rate 6.6 kmol/h with energy consumption 25.57 MW.

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Figure 3 Pareto set of maximization for hydrogen recovery rate and the minimization for energy consumption

Figure 3 shows the relation between hydrogen recovery rate and energy consumption. When maximization for hydrogen recovery rate and the minimization for energy consumption are simultaneously considered, corresponding to the feasible solution space, Pareto set concentrates in small areas. In the Pareto frontier, the compressor is only located in Position C or D. In the Pareto frontier, an approximate linear relationship can be seen between energy consumption and hydrogen recovery rate. It means the energy consumption requires 0.185 MW/kmol hydrogen recovery. In terms of the energy consumption, hydrogen recovery rate affects the energy consumption more than ethylene loss rate.



Figure 4 Pareto set of maximization for hydrogen recovery rate and the minimization for ethylene loss rate

Figure 4 shows the relation between hydrogen recovery rate and ethylene loss rate. Two levels with a step constitute the Pareto frontier. In each level, ethylene loss rate slightly rises with the increase of hydrogen recovery rate. The compressor can be located in Position B and Position C in the lower level while the compressor is located in position D in the upper level.



Figure 5 Pareto frontier of the triple-objective synthesis

Figure 5 shows the result of the triple-objective synthesis. It is a 3D Pareto frontier for the triple-objective optimization. As can be observed that, when the hydrogen recovery rate increases the ethylene loss rate also increases while the energy consumption decreases. In the single objective process synthesis, it has been proved that the operation temperature of the flash drums tend to stay upper boundary to increase the hydrogen recovery rate. On the one hand, the operation for the flash drums in a higher temperature saves the amount of refrigerant. On the other hand, the energy recycling also increases with the hydrogen recovery rate increases. Through the Figure 5, whether a trade-off solution or an extreme solution is selected depends on the decision makers or economic performance.

#### 4. Conclusions

The chilling train system in ethylene plants is regarded as an energy-induced separation networks (EISENs) in this dissertation. The single objective process synthesis models (minimize energy consumption only, minimize ethylene loss only, or maximize hydrogen recovery rate only) and the multi-objective process synthesis models (two objective process synthesis and triple objective process synthesis) are developed based on the modular framework methodology. The single objective process synthesis models are solved by the simulated annealing algorithm, and the best position for the compressor and operating conditions are determined. The relationship among ethylene loss rate or the hydrogen production rate and energy consumption are obtained when non-dominated sorting genetic algorithm-II (NSGA-II) is used.

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