Superstructure Optimization of the Olefin Separation Process

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Abstract

The olefin separation process involves handling a feed stream with a number of hydrocarbon components. The objective of this process is to separate each of these components at minimum cost. We consider a superstructure optimization for the olefin separation system that consists of several technologies for the separation task units and compressors, pumps, valves, heaters, coolers, heat exchangers. We model the major discrete decisions for the separation system as a generalized disjunctive programming (GDP) problem. The objective function is to minimize the annualized investment cost of the separation units and the utility cost. The GDP problem is reformulated as an MINLP problem, which is solved with the Outer Approximation (OA) algorithm that is available in DICOPT++/GAMS. The solution approach for the superstructure optimization is discussed and numerical results of an example are presented.

1. Introduction

The olefin process involves a number of steps for producing and separating hydrocarbon components consisting of hydrogen and C_1~C_5 components. We address the optimization of the separation system where the feed and the products are given. The goal is to select a configuration of separation tasks and their corresponding units, as well as pressure and temperature levels in order to perform heat integration. The objective is to minimize the total annualized cost of the separation system. Figure 1 shows the superstructure of the olefin separation system. There are number of states and separation tasks. The white boxes represent sharp split separations and the shaded boxes represent non-sharp split separations. We consider 8 components in the separation system and they are hydrogen, methane, and C_2~C_5 components. Since we are mainly concerned with the recovery of ethylene and propylene, we assume that the C_4 mixture and the C_5 mixture can be treated as a single component. As shown in Figure 1, there are 25 states including final products and 53 separation tasks. Non-sharp split separations have intermediate components which appear in both the top and bottom products. For each separation task, there is a subset of technologies available depending on the separation task. Table 1 shows 7 separation technologies considered in the separation process. Dephlegmator is a separation unit where heat exchange and mass transfer take place at the same time. Cold box is a cryogenic separation unit that is based on Joule-Thomson effect. Each separation task can be performed by a number of separation technologies, which are selected based on the components involved in the feeds.

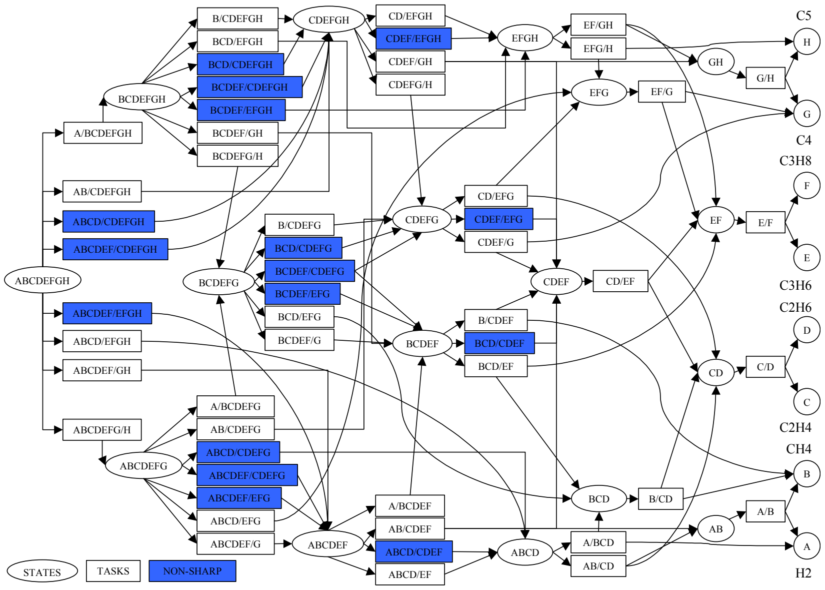

Figure 1: Superstructure of separation system

Table 1: Separation technologies

T1	Distillation column
T2	Physical absorption tower
T3	Membrane separator
T4	Dephlegmator
T5	Pressure Swing Adsorption (PSA)
T6	Cold Box
T7	Chemical Absorption tower

2. GDP model

We propose a generalized disjunctive programming model for optimizing the superstructure of the separation system shown in Figure 1 (see Yeomans and Grossmann, 1999a, 1999b). The first level in the embedded disjunction corresponds to the selection of the separation task. Once the separation task is selected, the second level disjunction is for the selection of the separation technologies. For example, if a distillation column is chosen, then the mass and energy balances for distillation column are enforced and the corresponding cost term is considered. An additional disjunction is the heat integration for the distillation columns, and another disjunction is for compression, pumping or pressure reduction of each state. For the separation units, simple mass/energy balances are used. Assumptions for modeling the separation system are as follows:

1) Vapor pressure of the stream is calculated with Raoult's law and by the Antoine equation (Reid et al., 1977)
2) Utility (cooling water/hot steam) cost is given by a function of temperature (see Figure 2)
3) Investment cost is given by concave cost functions (Douglas, 1988)

Based on these assumptions, the following nonconvex GDP model is constructed:

Indices

i	States	k	Distillation column
s	Separation task	st	Separation technology

Sets

I	States i	K	Distillation column k
S_i	Separation task s for state i	ST_s	Separation technology st for task s

Parameters

EMAT	Minimum T difference		
CR_L	Lower bound for comp. ratio	CR_U	Upper bound for comp. Ratio

Variables

x_i	Flowrate of state i	T_i	Temperature of state I
P_i	Pressure of state i	IC_i	Investment cost for separation of i
CC_i	Compressor cost for state i	UC_i	Utility cost for separation of I
$YS_{i,s}$	Selection of separation task	$YZ_{i,k}$	Selection of heat integration for state i
$YT_{s,st}$	Selection of separation tech.	YC_i	Selection of compression for state i
RT_i	Top recovery ratio of state i	RB_i	Bottom recovery ratio of state i
$QEX_{i,k}$	Heat transferred from state i to distillation column k		
Q_i	Heat generated or consumed by state I		
T_i^C	Condenser temperature in distillation column for I		
T_k^R	Reboiler temperature in distillation column k		

Model Olefin1:

a) Minimize the annualized cost of capital investment, compression and utility

$$\min Z = \sum_i \left(IC_i + CC_i + UC_i \right)$$

b) Overall mass balances

$$s.t. \quad Ax = 0$$

c) Pressure and temperature calculation by Antoine equation

$$P_i = fa(T_i), \quad \forall i \in I$$

d) Embedded disjunction for the separation task

$$\bigvee_{s \in S_i} \begin{bmatrix} YS_{i,s} \\ x_i^{top} = RT_i x_i^{feed} \\ x_i^{btm} = RB_i x_i^{feed} \\ \bigvee_{st \in ST_s} \begin{bmatrix} YT_{s,st} \\ mass\ balance: fm(x_i) = 0 \\ energy\ balance: fe(x_i, T_i, P_i, Q_i) = 0 \\ \cos t\ \ fuction: (IC_i, UC_i) = fc(x_i, T_i, P_i, Q_i) \end{bmatrix} \end{bmatrix}, \quad \forall i \in I$$

e) Disjunction for the heat integration

$$\begin{bmatrix} YZ_{i,k} \\ T_i^C \geq T_k^R + EMAT \\ QEX_{i,k} \geq 0 \\ (IC_i, UC_i) = fz(x_i, T_i, P_i, QEX_{i,k}) \end{bmatrix} \vee \begin{bmatrix} \neg YZ_{i,k} \\ QEX_{i,k} = 0 \end{bmatrix}, \quad \forall i \in I, \forall k \in K$$

f) Disjunction for the compressors/pumps

$$\begin{bmatrix} YC_i \\ (T_i, P_i)_{out} = fp_1(T_i, P_i)_{in} \\ CR_L \leq P_i^{out} / P_i^{in} \leq CR_U \\ CC_i = fp_2(x_i, T_i, P_i) \end{bmatrix} \vee \begin{bmatrix} \neg YC_i \\ (T_i, P_i\ )_{out} = (T_i, P_i)_{in} \\ CC_i = 0 \end{bmatrix}, \quad \forall i \in I$$

g) Logic propositions

$$\begin{array}{ll} \vee YS_{i,s} & \forall i \in I \\ YS_{i,s} \Rightarrow \vee YT_{s,st} & \forall st \in ST_s, \forall s \in S_i, \forall i \in I \\ \neg YS_{s,st} \Rightarrow \neg YZ_{i,k} & \forall st \in ST_s, \forall s \in S_i, \forall i \in I, \forall k \in K \end{array}$$

h) Variable bounds

$$\begin{array}{l} 0 \leq x_i \leq x^{UP}; T^{LO} \leq T_i \leq T^{UP}; P^{LO} \leq P_i \leq P^{UP}, \quad \forall i \\ 0 \leq RT_i, RB_i \leq 1 \qquad \forall i \\ 0 \leq IC_i, CC_i, UC_i \qquad \forall i \\ YS_{i,s}, YT_{s,st}, YZ_{i,k}, YC_i \in \{true, false\} \quad \forall i, s, st, k \\ 0 \leq Q_i, QEX_{i,k} \quad \forall i, k \\ T^{LO} \leq T_i^C, T_k^R \leq T^{UP} \quad \forall i, k \end{array}$$

In the above model *fa*, *fm*, *fe*, *fc*, *fz*, fp_1, and fp_2 are the corresponding functions for the calculation of pressure, mass balance, energy balance, investment and utility cost, heat exchange cost, and compressor/pump cost, respectively. We adopt simple model equations for the cost calculation of the process units and compressor T/P (Douglas 1988; Biegler et al., 1997). The above GDP model is transformed into an MINLP using the big-M formulation for the disjunctions (Lee and Grossmann, 2000).

3. Utility system

The process streams and separation units require individual cooling/heating for the temperature changes. We consider heat integration with a number of available utility streams with different temperature. Due to the discrete choices of the temperature and cost, the optimal selection of the utility stream yields a mixed-integer nonlinear model to select a specific utility stream. However, as shown in Figure 2, the utility cost can be approximated by a smooth function of the temperature. In this way, we can avoid introducing the binary variables and simplify the modeling of utility system. We construct a third order regression of the utility cost, which yields a good approximation. This approximation generally provides an underestimation of the actual cost of the utility streams because we introduce a continuous relaxation of the temperature levels of the utilities.

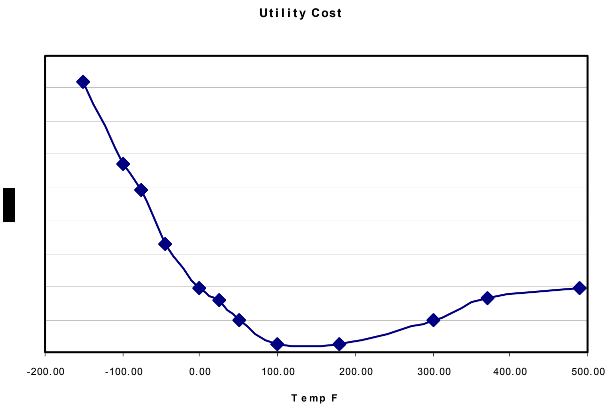

Figure 2: Utility stream temperature

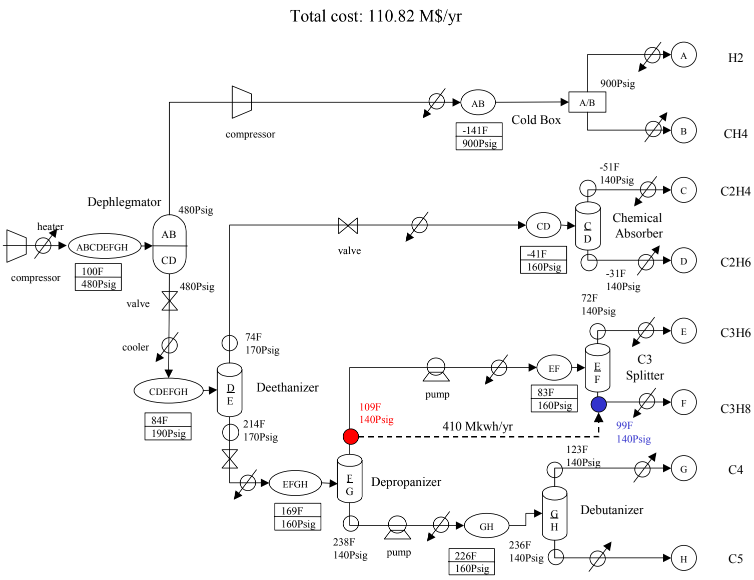

Figure 3: GAMS optimal solution

4. Numerical results

Figure 3 shows the optimal solution for the superstructure shown in Figure 1. First the compressors are used to increase the pressure of the feed stream to the dephlegmator, which separates the hydrogen and methane from the heavier components. Then the hydrogen/methane mixture is sent to the cold box and hydrogen is separated from methane. The cold box operates at the low temperature and high pressure which requires additional refrigeration and compression. The C_2-C_5 mixture is sent to the deethanizer (distillation column) and the C_2 mixture is recovered as top product. The C_3 mixture is separated by the depropanizer, and the C_4-C_5 mixture is sent to the debutanizer. A chemical absorber is used for the C_2 split and distillation column is used for the C_3 split. All the separation units perform sharp separations. Note that there is a heat exchange between the depropanizer and the C_3 splitter to reduce the utility cost. The annualized capital cost of the process is 39.1M$/yr. The power cost for the compressors is 29.8M$/yr and the utility cost for the separation units is 41.9M$/yr. The energy cost is about 75% of the total cost. Since the olefin separation process is highly energy-intensive, a significant amount of utility cost can be saved by the heat integration. Table 2 shows the statistics of the problem, where it can be seen that the MINLP problem is very large. This MINLP was solved in about 2 hours on a Pentium PIII PC using GAMS/DICOPT++, an algorithm for MINLP problems that is based on the Outer Approximation (OA) with Equality Relaxation and Augmented Penalty (Viswanathan and Grossmann, 1990). CPLEX was used for the MILP solver and CONOPT2 was used for the NLP solver in GAMS (release 20.7). The heuristic termination was used that is based on the lack of improvement in the objective.

Table 2: GAMS computational results

MINLP problem size		DICOPT++ solution	
Number of constraints	52,703	Number of iterations	5
Number of variables	24,475	CPU seconds	8,778
Number of binary variables	5,851	First integer solution	142.9 M$/yr

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Acknowledgments

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