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Optimal Synthesis of Ethylene Production Process

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This work addresses the energetic and economic optimization for the synthesis of distillation-based ethylene production. We employ a model-based optimization approach to determine the optimal sequencing of processes for olefins separation that involves handling a multicomponent mixture. The optimization model is formulated based on a superstructure that embeds many possible and feasible structural alternatives for processing a number of hydrocarbon components constituting gaseous ethane or liquid naphtha. We adopt linear mass balance reactor models for conversion of materials into desirable products and simple sharp distillation column models based on split fractions for product recovery from a multicomponent feed stream. The formulation leads to a mixed-integer linear program (MILP) with discrete 0–1 variables on task selection and continuous variables on input flowrate to each task. To aid convergence to the optimal system synthesis with minimum total annualized cost, the model incorporates heuristic-based logical constraints that represent design and structural specifications on engineering knowledge, design experience, and rules of thumb. The model is implemented on case studies drawn from actual operating petrochemical plants in Malaysia with reasonable computational results.

1. Introduction

There is a renewed interest in ethylene production in the US that is spurred by a significant shift in its raw material due to shale gas production. The latter revolution has yielded availability of low cost ethane and is driving a resurgence in the petrochemical industry in the US with repercussions to its other industries as well as energy and trade flows around the world. It is projected that by 2023, approximately 50 percent of global ethylene production will be from the gaseous feedstock of ethane and liquefied petroleum gas (LPG) with the remaining produced from the liquid feedstock of naphtha (Hydrocarbon Processing, 2013) and gasoil (van Goethem et al., 2013). The key technology in ethylene production centers around distillation, which remains an energy-intensive and high-cost operation. Hence, there is substantial economic incentive in optimally selecting the best separation sequence for a particular process. Puigjaner and Heyen (2006) and Caballero et al. (2009) report column sequencing as one of the most challenging synthesis problems in the chemical industry mainly due to the increasing number of structural alternatives. Application of heat integration technique has been reported for energy reduction in distillation-based processes (Ochoa-Estopier et al., 2013).

The rest of the paper is organized as follows. Section 2 formally describes the problem addressed in this work. Section 3 presents the proposed superstructure and MILP model formulation to handle the problem. Section 4 reports the model implementation and discusses the results before concluding.

2. Problem statement

We address the optimal processing sequence of an olefins mixture given data on the composition and total feedstock flowrate (as based on product yields from a thermal cracking unit for naphtha or ethane), the availability and maximum capacity of process units, utility cost, and product demands. We wish to determine the continuous variables on stream flow rates and the 0–1 variables on selection of tasks that satisfy minimum total annualized cost. A model-based superstructure optimization approach is employed by adopting linear mass balance reactor models for conversion of materials into desirable products. Each

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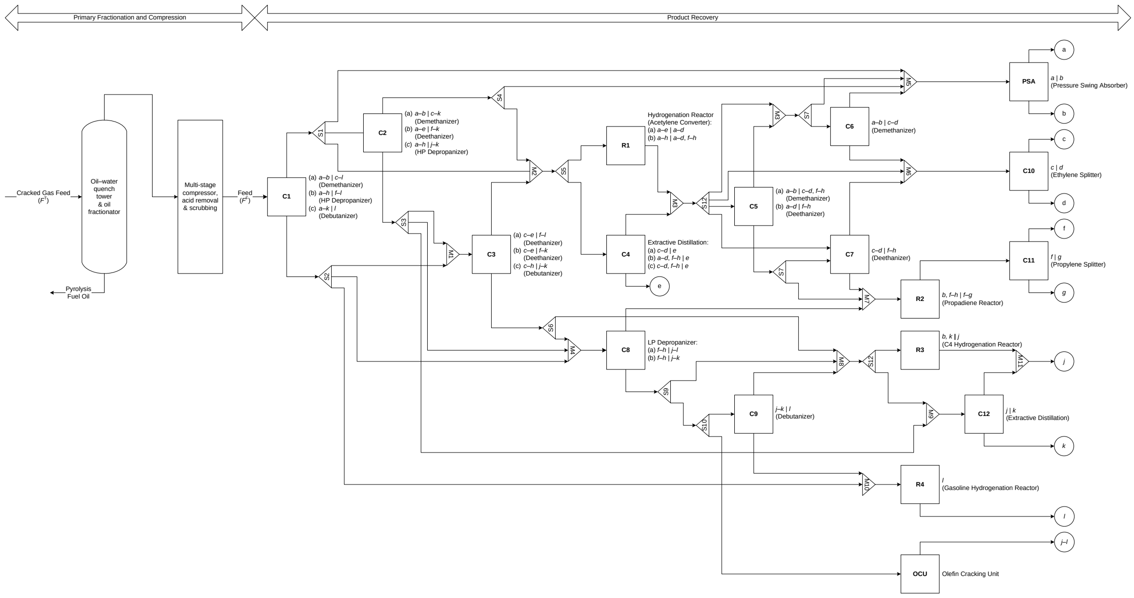

Figure 1: Intermediate superstructure representation for the processing sequence of an olefins mixture

of the distillation columns is assumed to perform simple split involving one feed and two products consisting of distillate and bottoms as well as sharp separation in which an entering component leaves in only one product stream, which gives rise to complete (100 %) recovery.

3. Mathematical formulation

A model-based optimization approach is employed to determine the optimal processing sequence of a multicomponent olefins mixture. The optimization model is formulated based on a superstructure that embeds many possible and feasible structural alternatives for processing a number of hydrocarbon components constituting gaseous ethane or liquid naphtha. We adopt linear mass balance reactor models for conversion of materials into desirable products (Biegler et al., 1997) and simple sharp distillation column models based on split fractions for product recovery from a multicomponent feed stream (Andrecovich and Westerberg, 1985).

3.1 Superstructure representation

We adopt an intermediate superstructure representation for the processing sequence of an olefins mixture as shown in Figure 1. Such a representation leads to a smaller model formulation than a more conventional state–task network representation (Caballero and Grossmann, 1999). For a distillation column, a feed stream is separated into two products streams, namely distillate and bottoms. Details on the legend for the superstructure are provided in Table 1 in Section 4.

3.2 Model constraints

The material balances describe material flows into and out of a task for a distillation column or a reaction in the superstructure. Each intermediate component i produced by a task equals the amount of that component i fed to a task that further reacts or separates the component:

$$\sum_{j \in J_i^{\mathrm{G}}} \xi_j^i F_j = \sum_{j \in J_i^{\mathrm{H}}} F_j, \quad i \in I \tag{1}$$

where F_j is the feed flow rate to a task j, ξ_j^i is the split fraction of component i in task j, J_i^{G} is the set of all tasks j producing a known component i, J_i^{H} is the set of all tasks j having intermediate component i as feed, and I is the set of all intermediate components. The balance is written for each intermediate component.

For the initial node of the network:

$$F^{\mathrm{T}} = \xi_{\mathrm{A}}^{a-l} F_{\mathrm{A}} + \xi_{\mathrm{B}}^{m} F_{\mathrm{B}} \tag{2}$$

where F^{T} is the total flowrate of the cracked gas feed, F_{A} is the feed flow rate to task A performed by the oil–water quench tower, F_{B} is the feed flow rate to task B performed by the oil fractionator.
The feed to the main reaction and separation distillation system is described by:

$$\xi_{\mathrm{A}}^{a-l} F_{\mathrm{A}} = F^{\mathrm{F}} \tag{3}$$

where the flowrate F^{F} of the initial mixture to be processed is equal to the sum of the feed to each task that processes some portion of the mixture as given by:

$$F^{\mathrm{F}} = \sum_{j \in J_i^{\mathrm{F}}} F_j \tag{4}$$

where J_i^{F} is the set of all tasks *j* having the initial mixture as feed.

Switching constraints are imposed to ensure that non-existence of a task corresponds to zero input flow to the task. We consider a big-*M* formulation for such logical constraints that relate the continuous flowrate variables and the integer 0–1 variables on task selection as follows:

$$F_j \le M_j y_j, \quad \forall j \in J \tag{5}$$

Non-negativity constraints on the continuous variables:

$$F_j \ge 0, \quad \forall j \in J \tag{4}$$

Integrality constraints on the 0–1 variables:

$$y_j \in \{0,1\}, \quad \forall j \in J \tag{4}$$

3.3 Heuristic-based cuts

Heuristic-based cuts are incorporated in the formulation to aid convergence to optimality. The logic cuts serve to stipulate design specifications as based on engineering knowledge and past design experience as well as to enforce structural specifications on interconnectivity relationships among the component streams and tasks in the superstructure (Raman and Grossmann, 1991).
The logic cut on design specification for the tasks processing the initial mixture enforces that exactly one of the available tasks is selected:

$$\sum_{j \in J_i^{\mathrm{F}}} y_j = 1 \tag{6}$$

The logic cut on design specifications for the tasks that produce intermediate components stipulate that at most one of the tasks associated with a piece of equipment is selected:

$$\sum_{j \in J_i^{\mathrm{F}}} y_j = 1 \tag{7}$$

The logic cuts on structural specifications apply to the distillate and bottoms of the distillation columns as well as reactor products as follows:

$$y_j \le \sum_{j \in J_i^{\mathrm{O}}} y_j, \quad \forall (i,j) \in \mathrm{IJ} \tag{8}$$

where $\mathbf{IJ}$ the set of all pairs of tasks *i* and their associated products *j* (both distillate and bottoms in the case of distillation columns),

3.4 Objective function

The objective function involves minimizing the total annualized processing costs that consist of the fixed investment cost and variable operating cost:

$$\min \sum_{j \in J} \left(\frac{1}{L} \mathrm{CC}_j y_j + \mathrm{OC}_j F_j H \right) \tag{9}$$

where L is the plant life (year), CC_j is the capital cost for purchasing and installing a piece of equipment associated with task j, OC_j is the cost of operating a task j, and H represents hours of plant operation per annum.

4. Case Studies

The formulated model is implemented on two case studies with data drawn from actual operating petrochemical plants in Malaysia. For the first case study, we consider a feed composition based on the yields of a gas cracking process of a gaseous ethane feedstock obtained from an ethylene plant producing polyethylene in the Kertih Integrated Petrochemical Complex in Malaysia. In the second case study, we consider the feed composition based on the thermal cracking yields of a liquid naphtha feedstock obtained from an ethylene plant in southern West (Peninsular) Malaysia. The respective composition for the two feedstock in weight percentage (wt%) is given in Table 1 (the key in column 1 refers to a component *i*).

Table 1: Feed compositions based on thermal cracking yields of ethane and naphtha feedstock

Key	Compound	Composition (wt%)for ethane feedstock	Composition (wt%)for naphtha feedstock
a	Methane (CH_4)	3.1	15.3
b	Hydrogen (H_2)	3.4	0.8
c	Ethane (C_2H_6)	46.0	3.8
d	Ethylene (C_2H_4)	42.5	29.3
e	Acetylene (C_2H_2)	0.1	0.7
f	Propane (C_3H_8)	0.2	0.3
g	Propylene (C_3H_6)	1.4	14.1
h	Propadiene (C_3H_4)	0.0	1.1
j	Butadiene (1,3-C_4H_6)	0.9	4.8
k	Butene (C_4H_8), Butane (C_4H_{10})	0.6	4.5
l	Pyrolysis gasoline	1.8	21.0
m	Fuel oil	0.1	3.8

The results of the processing sequences obtained are shown in Figure 2 for the optimal (best possible) solution while Figure 3 depicts the second best solution obtained by incorporating an appropriate integer cut in the model implementation. An optimal solution entails the lowest total mass flow rate hence the lowest total annualized cost, which is consistent with established heuristics (Douglas, 1988). While the second best sequence has two extra columns, it offers a wide range of products produced. It is worth noting that a relatively high ethylene production (from tasks C3a and C3b) and a low acetylene production due to ethane cracking gives rise to a need for task C4a.

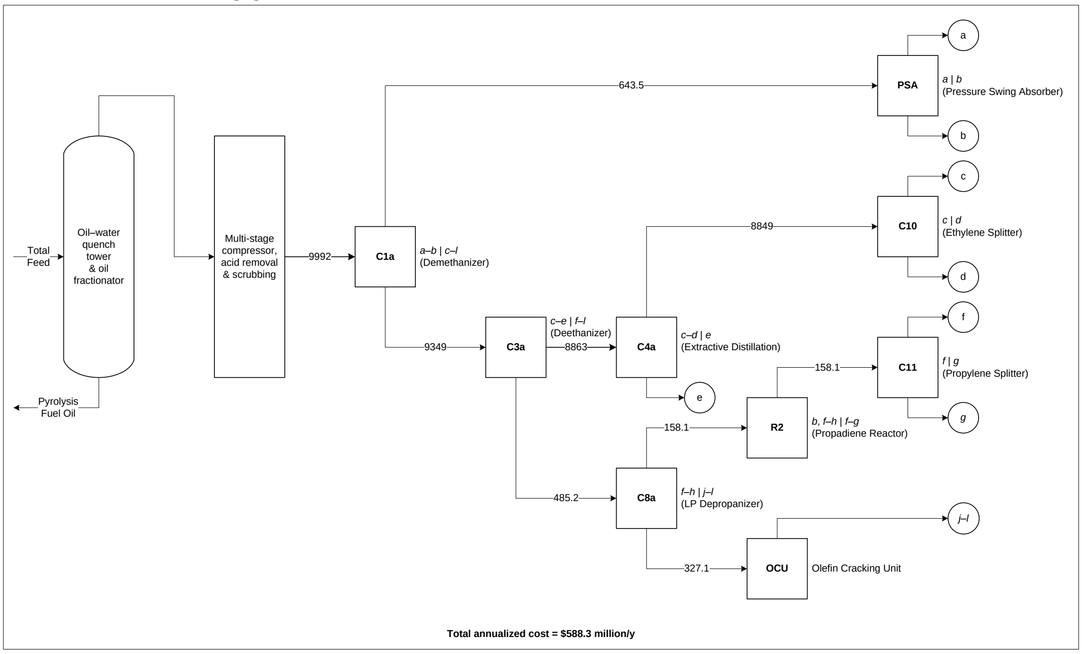

Figure 2: Optimal (best possible) solution for processing sequence of an ethane feedstock

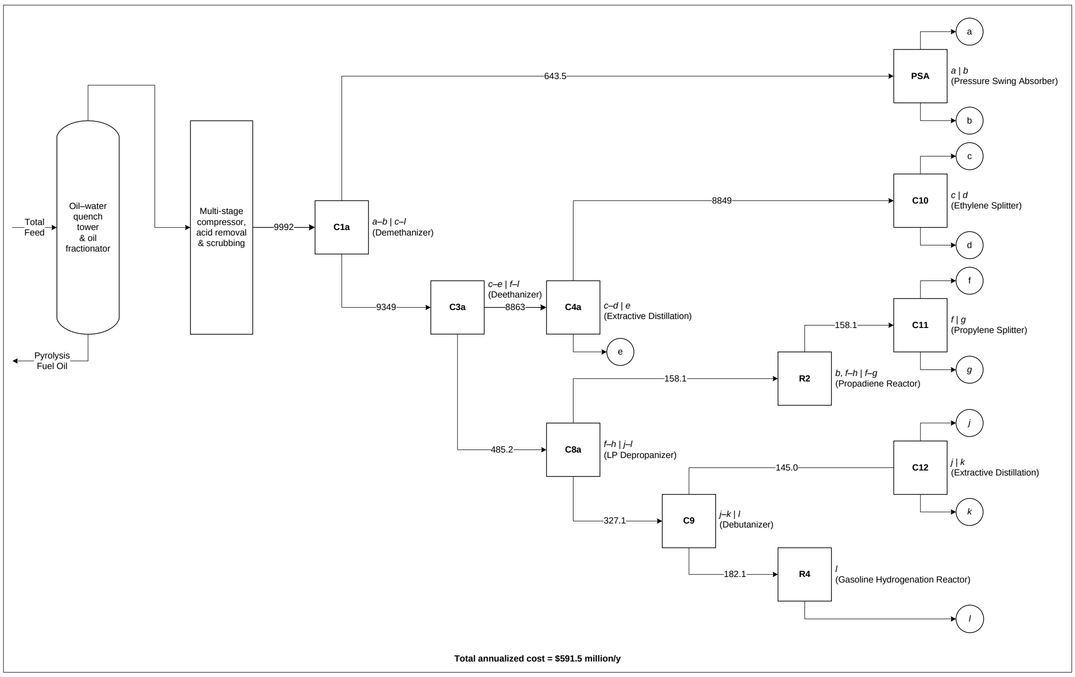

Figure 3: Second best solution for processing sequence of an ethane feedstock (obtained with use of integer cuts)

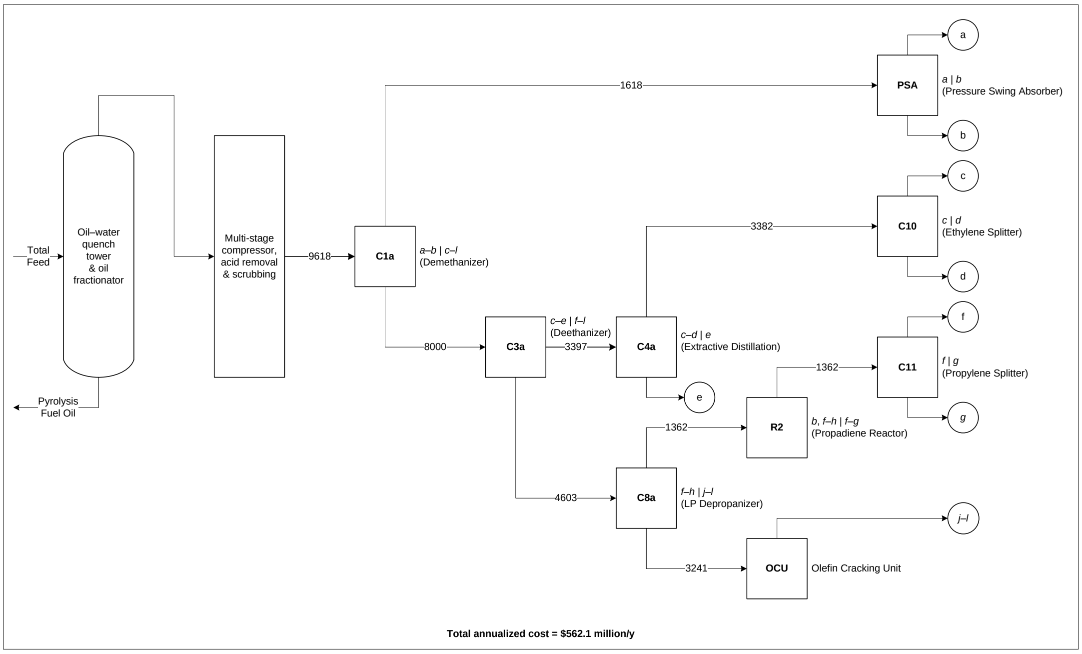

Figure 4: Optimal (best possible) solution for processing sequence of a naphtha feedstock

The results of the processing sequences of a naphtha feedstock are shown in Figure 4 for the optimal solution and Figure 5 for the second best solution. Similar to the results for an ethane feedstock, the best sequence entails the lowest total mass flowrate, which is a feature consistent with a heuristic of selecting a sequence with minimum total flows (Douglas, 1988). Such a characteristic also contributes to the lowest operating cost and in this case, to the lowest total annualized cost because fewest columns are selected, which attributes to the lowest capital cost. On the other hand, the second best sequence has two extra columns that lead to a wide range of products produced. The third best sequence registers the highest total cost because it involves the largest total flows—moreover, relatively high acetylene and low ethylene

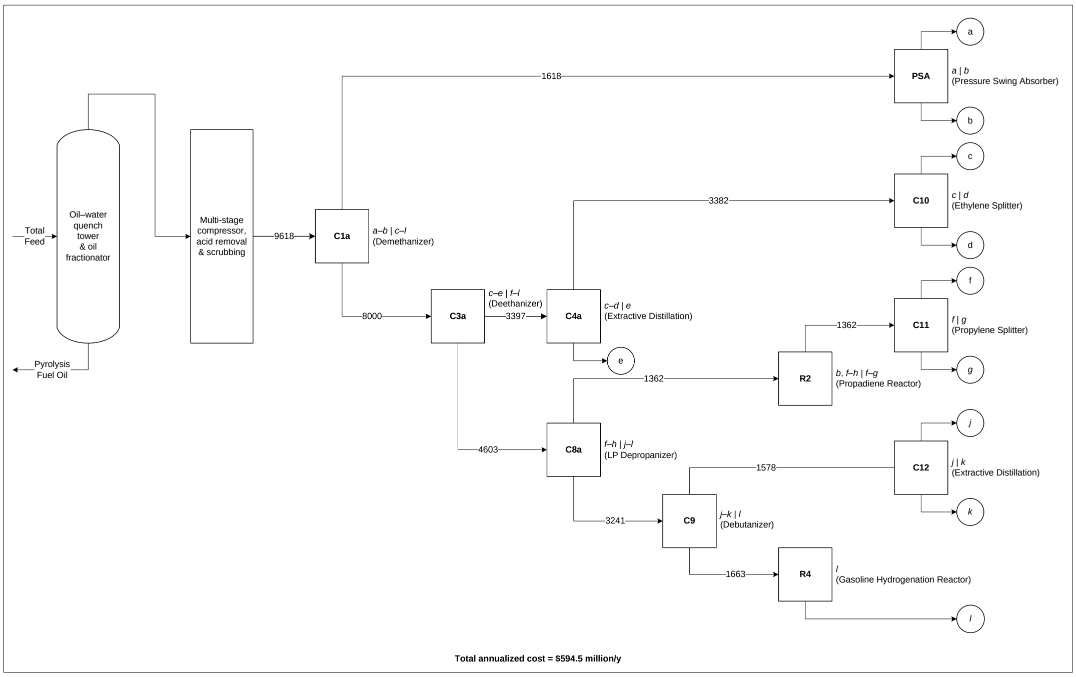

Figure 5: Second best solution for processing sequence of a naphtha feedstock (obtained with use of integer cuts)

production in this sequence entail the use of a catalytic hydrogenation reactor to convert acetylene to ethylene.

The processing sequence for an ethane feedstock offers a higher ethylene yield as compared to that for a naphtha feedstock. This increases the total annualized cost because separating ethylene from ethane requires a large number of stages in a distillation column. Ethylene is a profitable product but requires a high production cost.

5. Conclusions

This work presents an MILP model formulation to optimize processing sequence of an olefins mixture for ethylene production. The results obtained show good agreement with established heuristic on case studies based on actual operating plants.

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