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Optimization of Petroleum Refinery Configuration Design with Logic Propositions

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***Abstract*—**This work concerns the topological optimization problem for determining the optimal petroleum refinery configuration. We are interested in further investigating and hopefully advancing the existing optimization approaches and strategies employing logic propositions to conceptual process synthesis problems. In particular, we seek to contribute to this increasingly exciting area of chemical process modeling by addressing the following potentially important issues: (a) how the formulation of design specifications in a mixed-logical-and-integer optimization model can be employed in a synthesis problem to enrich the problem representation by incorporating past design experience, engineering knowledge, and heuristics; and (b) how structural specifications on the interconnectivity relationships by space (states) and by function (tasks) in a superstructure should be properly formulated within a mixed-integer linear programming (MILP) model. The proposed modeling technique is illustrated on a case study involving the alternative processing routes of naphtha, in which significant improvement in the solution quality is obtained.

***Keywords*—**Mixed-integer linear programming (MILP), petroleum refinery, process synthesis, superstructure.

I. Introduction

PROCESS synthesis or conceptual process design is concerned with the identification of the best flowsheet structure to perform a given task. Three major approaches are traditionally available in the literature to address this class of problem: (1) the heuristics method, notably the hierarchical decomposition of design decisions procedure of Douglas [1]; (2) the technique based on thermodynamic targets and physical insights, as exemplified by pinch analysis [2]; and (3) the algorithmic approach, which utilizes optimization, based on the construction of a superstructure that seeks to represent all feasible process flowsheets [3]. This work aims to extend the superstructure-optimization-based approach of using logic cuts, as proposed by [4]–[7], to incorporate qualitative design knowledge based on engineering experience and heuristics in modeling the major process flows in a refinery.

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II. Problem Statement

We consider the following process synthesis problem of superstructure optimization for the topology design of a refinery. Given the following data: (a) fixed production amounts of desired products; (b) available process units and ranges of their capacities; (c) cost of crude oil and cost structure for process units; determine the optimal topology or configuration of the refinery in terms of: (a) the selection and sequencing of the streams and (b) the stream flowrates.

III. Propositional Logics and Logic Cuts in Process Synthesis Problems

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IV. Propositional Logics and Logic Cuts in Process Synthesis Problems

This work is based on the mixed-integer linear program of [8] for determining the optimal topology of a refinery with environmental considerations. The emphasis here is an extensive investigation of employing logic cuts of logical constraints on the design and structural specifications of a refinery design. Logic cuts serve to reduce the computational expense of solving an MILP by tightening its linear relaxation and excluding fractional solutions [9]. They are linear inequalities or equalities formulated by using 0–1 variables to represent discrete decisions for the selection of alternative tasks corresponding to the process units i, as represented by the 0–1 variables y_i, and alternative states corresponding to the material streams j, as represented by the 0–1 variables z_j.

V. Superstructure Optimization Model Formulation for the Subsystem of Naphtha Produced from the Atmospheric Distillation Unit (ADU)

Figure 1 shows a state–task network (STN)-based superstructure representation that is sufficiently rich to embed all possible alternative topologies for the subsystem of naphtha produced from the atmospheric distillation unit

(ADU) of a refinery. Constant-yield material balances are employed to represent the process units, mainly in order to preserve the model linearity (for an MILP formulation).

A. Description of Superstructure

Based on the depicted superstructure of processing alternatives for naphtha exiting the ADU in Figure 1, we consider the following design specification: “MIX–3 is selected if and only if LSRN–1 or LSRN–3 is produced”. We contemplate the use of two logical relations and comment on some possible pitfalls.

First, using a combination of the logical “or” operator and the “equivalence” logic relation in the following form:

$$\left(Z_{\mathrm{LSRN-1}} \vee Z_{\mathrm{LSRN-3}}\right) \Leftrightarrow Y_{\mathrm{MIX-3}} \tag{1}$$

This is equivalent to the following two logic propositions:

$$\begin{aligned} &\left(Z_{\mathrm{LSRN-1}} \vee Z_{\mathrm{LSRN-3}}\right) \Rightarrow Y_{\mathrm{MIX-3}} \\ &Y_{\mathrm{MIX-3}} \Rightarrow \left(Z_{\mathrm{LSRN-1}} \vee Z_{\mathrm{LSRN-3}}\right) \end{aligned} \tag{2}$$

By employing the following steps involving the De Morgan’s theorem, these yields:

$$\begin{aligned} &\left(Z_{\mathrm{LSRN-1}} \vee Z_{\mathrm{LSRN-3}}\right) \Rightarrow Y_{\mathrm{MIX-3}} \\ &\neg\left(Z_{\mathrm{LSRN-1}} \vee Z_{\mathrm{LSRN-3}}\right) \vee Y_{\mathrm{MIX-3}} \\ &\left(\neg Z_{\mathrm{LSRN-1}} \wedge \neg Z_{\mathrm{LSRN-3}}\right) \vee Y_{\mathrm{MIX-3}} \\ &\underbrace{\left(\neg Z_{\mathrm{LSRN-1}} \vee Y_{\mathrm{MIX-3}}\right)}_{\substack{1-z_{\mathrm{LSRN-1}}+y_{\mathrm{MIX-3}}\geq 1 \\ y_{\mathrm{MIX-3}}\geq z_{\mathrm{LSRN-1}}}} \wedge \underbrace{\left(\neg Z_{\mathrm{LSRN-3}} \vee Y_{\mathrm{MIX-3}}\right)}_{\substack{1-z_{\mathrm{LSRN-3}}+y_{\mathrm{MIX-3}}\geq 1 \\ y_{\mathrm{MIX-3}}\geq z_{\mathrm{LSRN-3}}}} \end{aligned} \tag{3}$$

$$\begin{aligned} &Y_{\mathrm{MIX-3}} \Rightarrow \left(Z_{\mathrm{LSRN-1}} \vee Z_{\mathrm{LSRN-3}}\right) \\ &\neg Y_{\mathrm{MIX-3}} \vee \left(Z_{\mathrm{LSRN-1}} \vee Z_{\mathrm{LSRN-3}}\right) \\ &\left(1-y_{\mathrm{MIX-3}}\right) + z_{\mathrm{LSRN-1}} + z_{\mathrm{LSRN-3}} \geq 1 \\ &z_{\mathrm{LSRN-1}} + z_{\mathrm{LSRN-3}} \geq y_{\mathrm{MIX-3}}. \end{aligned} \tag{4}$$

Thus, we obtain the following algebraic constraints:

$$\begin{aligned} y_{\mathrm{MIX-3}} &\geq z_{\mathrm{LSRN-1}} \\ y_{\mathrm{MIX-3}} &\geq z_{\mathrm{LSRN-3}} \\ z_{\mathrm{LSRN-1}} + z_{\mathrm{LSRN-3}} &\geq y_{\mathrm{MIX-3}} \end{aligned} \tag{5}$$

However, the pitfall to using this formulation is that it allows the 0–1 variables to be satisfied for the case of ($z_{\mathrm{LSRN\ 1}}$, $z_{\mathrm{LSRN\ 3}}$, $y_{\mathrm{MIX\ 3}}$) = (1, 1, 1). This violates the physics of the problem stipulating that either LSRN–1 or LSRN–3 (only) is selected in the optimal configuration.

Second, consider now the use of the logical relation “exclusive 'or'” as given by the following:

$$\left(Z_{\mathrm{LSRN-1}} \veebar Z_{\mathrm{LSRN-3}}\right) \Leftrightarrow Y_{\mathrm{MIX-3}} \tag{6}$$

Translating this logic proposition into its equivalent algebraic constraints form, the proposition corresponds to:

$$\begin{aligned} &z_{\mathrm{LSRN-1}} + z_{\mathrm{LSRN-3}} = y_{\mathrm{MIX-3}} \\ &z_{\mathrm{LSRN-1}} + z_{\mathrm{LSRN-3}} = 1 \end{aligned} \tag{7}$$

However, there are three possible pitfalls in the use of this logical relation, which are all attributable to the logical constraint (8). First, this constraint compels either LSRN–1 stream or LSRN–3 stream to be selected even if there is no crude oil feed. Second, the two linear inequalities (7) and (8) enforce that $y_{\mathrm{MIX-3}}$ = 1, which mandates the MIX–3 unit to be selected under all circumstances—in other words, it requires MIX–3 to be a permanent feature of a refinery topology, which violates the physical problem. Third, this logic proposition is *not* satisfied for the case of ($z_{\mathrm{LSRN-1}}$, $z_{\mathrm{LSRN-3}}$, $y_{\mathrm{MIX-3}}$) = (0, 0, 0), which is the hypothetical case of no crude oil feed is available.

Thus, the constraints given by (5) best enforce the design specification that “MIX 3 is selected if and only if LSRN–1 or LSRN–3 is produced”.

B. General Formulation of a Class of Potentially Useful Logical Constraints

In our computational experiments, it is perhaps noteworthy to highlight the following frequently-encountered form of logic proposition in developing logical constraints on design specifications and structural specifications for synthesis problems. The logic form is generally given as:

$$\bigvee_{k=1,2,\cdots,M} Y_{u,k} \Leftrightarrow Y_u \qquad \forall u \in U = \{1, 2, \cdots, N\} \tag{8}$$

which is equivalent to:

$$\left(\bigvee_{k=1,2,\cdots,M} Y_{u,k} \Rightarrow Y_u\right) \wedge \left(Y_u \Rightarrow \bigvee_{k=1,2,\cdots,M} Y_{u,k}\right), \quad \forall u \in U \tag{9}$$

Transforming these logic propositions into inequalities yields:

$$\begin{aligned} &\bigvee_{k=1,2,\cdots,M} Y_{u,k} \Rightarrow Y_u && \forall u \in U \\ &Y_{u,k} \Rightarrow Y_u && \forall u \in U, k = 1, 2, ..., M \\ &\neg Y_{u,k} \vee Y_u && \forall u \in U, k = 1, 2, ..., M \\ &\left(1-y_{u,k}\right) + y_u \geq 1 && \forall u \in U, k = 1, 2, ..., M \\ &y_u - y_{u,k} \geq 0 && \forall u \in U, k = 1, 2, ..., M \end{aligned} \tag{10}$$

and:

$$\begin{aligned}
&Y_u \Rightarrow \underset{k=1,2,\cdots,M}{\vee} Y_{u,k} && \forall u \in U \\
&\neg Y_u \vee \left(\underset{k=1,2,\cdots,M}{\vee} Y_{u,k} \right) && \forall u \in U \\
&\left(1 - y_u\right) + \sum_{k=1}^{M} y_{u,k} \geq 1 && \forall u \in U \\
&\sum_{k=1}^{M} y_{u,k} - y_u \geq 0 && \forall u \in U
\end{aligned} \tag{11}$$

C. Extensive Logic Cuts for Processing Alternatives of Naphtha

In summary, the following are the rest of the complete set of logical statements and their associated logic propositions for the subsystem of naphtha produced from ADU. Due to space constraint, we use the abbreviations "iff" to denote "if and only if" and "i-s" to denote "is/are selected". Parentheses are used to improve readability.

- (HDT−1 or HDT−2) i-s iff ADU i-s: $Y_{\text{ADU}} \Leftrightarrow \left(Y_{\text{HDT}-1} \veebar Y_{\text{HDT}-2}\right)$
- SRU i-s iff (HDT−1 or HDT−2) i-s: $\left(Z_{\text{H2S}-1} \veebar Z_{\text{H2S}-2}\right) \Leftrightarrow Y_{\text{SRU}}$
- MIX–4 i-s iff (HSRN–3 or HSRN–4) i-s: $\left(Z_{\text{HSRN}-3} \vee Z_{\text{HSRN}-4}\right) \Leftrightarrow Y_{\text{MIX}-4}$
- MIX–5 i-s iff (NAP–3 or NAP–4) i-s: $\left(Z_{\text{NAP}-3} \vee Z_{\text{NAP}-4}\right) \Leftrightarrow Y_{\text{MIX}-5}$
- (MIX–3 and MIX–4), or (MIX–3 and MIX–5), or MIX–5 i-s iff (HDT–1 or HDT–2) i-s: $\left(Y_{\text{HDT}-1} \vee Y_{\text{HDT}-2}\right) \Leftrightarrow \begin{pmatrix} \left(Y_{\text{MIX}-3} \wedge Y_{\text{MIX}-4}\right) \vee \left(Y_{\text{MIX}-3} \wedge Y_{\text{MIX}-5}\right) \\ \vee Y_{\text{MIX}-5} \end{pmatrix}$
- REFu i-s iff (HSRN–5 or NAP–5) i-s: $\left(Z_{\text{HSRN}-5} \veebar Z_{\text{NAP}-5}\right) \Leftrightarrow Y_{\text{REFu}}$
- LPG i-s iff (HDT 1 or HDT 2) i-s: $\left(Y_{\text{HDT}-1} \vee Y_{\text{HDT}-2}\right) \Leftrightarrow Y_{\text{LPG}}$
- FGH i-s iff (FG–1 or FG–2 or FG–3 or FG–4) i-s: $\left(Z_{\text{FG}-1} \vee Z_{\text{FG}-2} \vee Z_{\text{FG}-3} \vee Z_{\text{FG}-4}\right) \Leftrightarrow Y_{\text{FGH}}$
- ISO i-s iff HDT–1 i-s: $Y_{\text{ISO}} \Leftrightarrow Y_{\text{HDT}-1}$

VI. Computational Results

A case study is undertaken using GAMS/CPLEX to implement the logic cuts for a light crude charge input (API gravity > 33°). The shaded units and streams in Figure 1 denote the optimal refinery topology computed, which reasonably agrees with real-world existing refinery configuration. In our computational experiments, the inclusion of the proposed cuts has been shown to improve the solution quality by cutting off suboptimal solutions that violate the important design and structural specifications enforced by the cuts.

VII. Concluding Remarks

This work attempts to extend the existing optimization modeling strategies of integrating qualitative-based information in synthesis problems by using logic cuts. In addition, some insights are provided on how to identify possibly inconsistent integer constraints derived from logic propositions. Also, in the case study, the selection of streams is considered as discrete decisions to determine the optimal topology. An immediate extension of this work is to investigate the computational performance of representing the logic propositions via disjunctions within the Generalized Disjunctive Programming framework [10].

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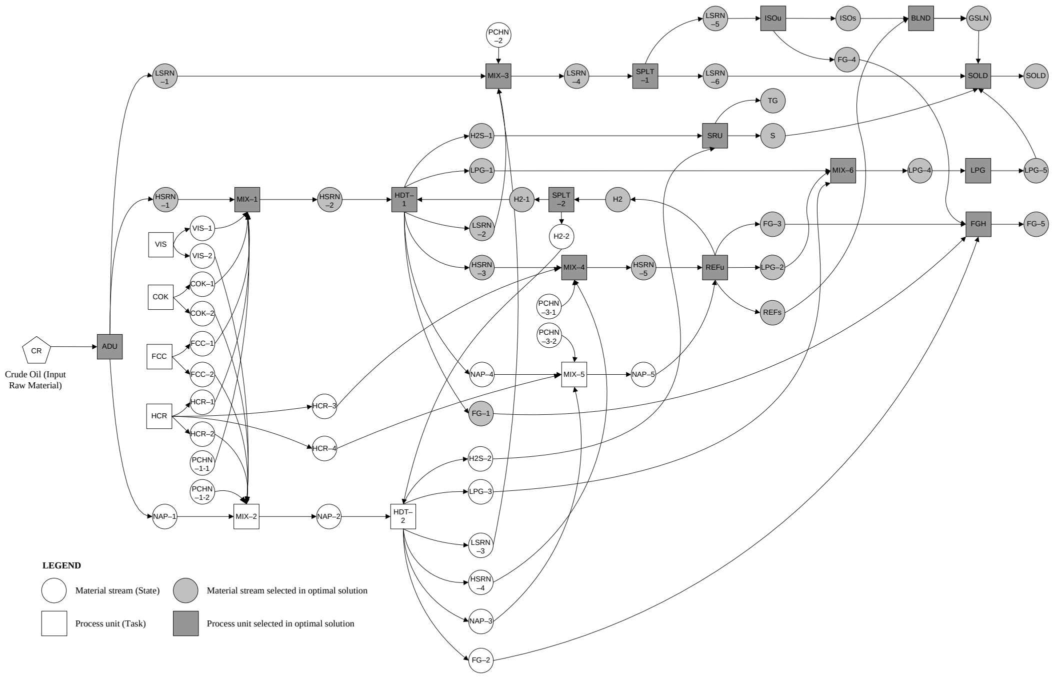

Fig. 1 STN-based superstructure of refinery topology for the naphtha subsystem (note: the shaded symbols represent the streams and units that are selected in the optimal solution for the case study on light crude oil charge)