Journal of Applied Sciences

ISSN 1812-5654

Journal of Applied Sciences 11 (21): 3571-3578, 2011
ISSN 1812-5654 / DOI: 10.3923/jas.2011.3571.3578

Optimal Design of Petroleum Refinery Topology using a Discrete Optimization Approach with Logical Constraints

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Abstract: This study proposes a logic-based modeling approach within a mixed-integer superstructure optimization framework on the topological optimization problem of determining the optimal configuration of a petroleum refinery. We are interested in further investigating and advancing the existing optimization approaches and strategies of employing logical constraints to conceptual process synthesis problems within the frameworks of the conventional Mixed-Integer Linear Program (MILP) and the alternative Generalized Disjunctive Program (GDP). In particular, we intend to address the following issues: (a) how the formulation of design specifications in a synthesis problem can be accomplished using logical constraints in a mixed-logical-and-integer optimization model to enrich the problem representation by way of incorporating past design experience, engineering knowledge and heuristics and (b) how structural specifications on the interconnectivity relationships by space (states) and by function (tasks) should be properly formulated using logical constraints within a mixed-integer optimization model. The proposed modeling technique is illustrated on a case study involving the alternative processing routes of naphtha in a refinery.

Key words: Design specifications, structural specifications, MILP, GDP, configuration, process synthesis

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; (2) the technique based on thermodynamic targets and physical insights as exemplified by pinch analysis and (3) the algorithmic approach that utilizes optimization based on the construction of a superstructure that seeks to represent all feasible process flowsheets (Seider *et al.*, 2009).

The intricate complexities associated with process synthesis problem in general and the refinery design problem in specific necessitates the development and implementation of a systematic and automated approach that efficiently and rigorously integrate the elaborate interactions involving the design decision variables. This study aims to extend the superstructure-optimization-based approach of using logical constraints (Raman and Grossmann, 1991, 1992, 1993, 1994) within a Mixed-Integer Linear Program (MILP) to incorporate qualitative design knowledge based on engineering experience and heuristics in modeling the major process flows in a refinery. These constraints adopt discrete integer decision variables of the binary 0-1 type to model the existence of a refinery process unit and the associated stream piping interconnections (which are effectively pipelines) in a network structure, in which a value of one for a 0-1 variable designates that a unit is present in the optimal structure while the converse is true for a value of zero. Our work serves to further substantiate that the use of 0-1 decision variables offer a more natural and powerful modeling approach compared to the conventional linear programming technique that employs only continuous decision variables (Hassan *et al.*, 2011; Adeosun and Adetunde, 2008; Lan, 2008; Lan *et al.*, 2008). It also affords the convenience of representing fixed-cost charges in the objective function formulation. A variation in the use of integer variables in optimization model formulations has been reported elsewhere (Nja and Udofia, 2009).

PROBLEM STATEMENT

We consider the following process synthesis problem of superstructure optimization for the topology design of a refinery. Given the following data:

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(a) fixed production amounts of desired products (b) the available process units and ranges of their capacities and (c) cost of crude oil and cost structure for process units, we are to determine the optimal topology or configuration of the refinery in terms of the selection and sequencing of the streams as well as the operating levels as represented by the stream flowrates.

PROPOSITIONAL LOGICS AND LOGIC CUTS IN PROCESS SYNTHESIS PROBLEMS

This study is based on the Mixed-Integer Linear Program (MILP) of Khor and Elkamel (2010) for determining the optimal topology of a refinery with environmental considerations. Our emphasis is to conduct an extensive investigation of employing logical constraints on the design and structural specifications of a refinery topology design. Logical constraints have been proven to be logic cuts that serve to reduce the computational expense of solving an MILP by tightening its linear relaxation and excluding fractional solutions without affecting the quality of the optimal solution (Hooker *et al*., 1994). They are algebraic linear inequalities or equalities formulated by using 0-1 binary variables to represent discrete decisions for the selection of alternative tasks corresponding to the process units as well as alternative states corresponding to the material streams.

SUPERSTRUCTURE OPTIMIZATION FOR 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 (ADU) of a refinery. A substantial part of the data and information for the associated case study is provided by a refinery in Malaysia through an industrial collaboration that took place in August-December 2008.

Process description for superstructure development: The first processing step in petroleum refining is crude distillation, in which Crude Oil (CR) is distilled into oil fractions with respect to its boiling points. Naphtha constitutes the lighter fractions that are obtained from this process. Depending on the distillation column design as well as the refinery economics, the ADU can produce: (a) light straight run naphtha (LSRN-1) and heavy straight run naphtha (HSRN-1) or (b) an undifferentiated class of naphtha, typically termed as wild Naphtha (NAP-1), for which the 0-1 structural variables of z_i are used to represent these three possible states of naphtha.

In the first case, LSRN-1 is mixed with purchased naphtha (PCHN-2) and LSRN-2 from the hydrotreater HDT-1 in a mixer (MIX-3). The output from MIX-3, i.e.,

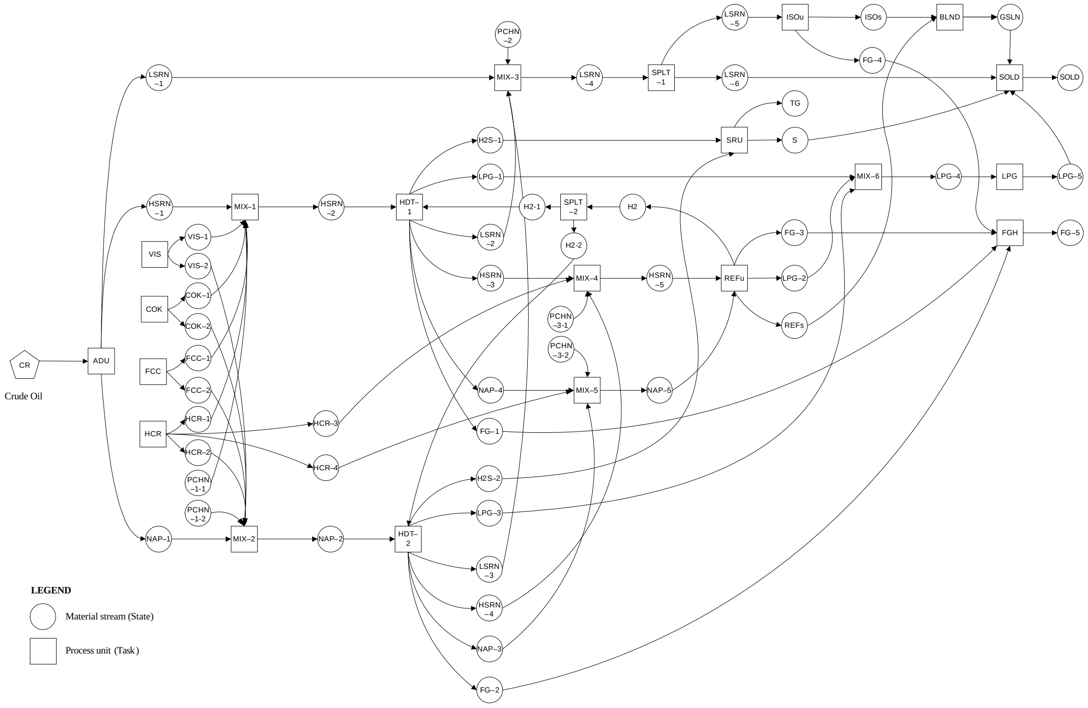

Fig. 1: STN-based superstructure representation on case study of refinery topology for naphtha processing subsystem

LSRN-4, can undergo two processes: (a) it is used as a feedstock for the Isomerization Unit (ISO) and (b) it is sold as a final product. Isomerization Yields Isomerate (ISO), one of the blending components for gasoline (GSLN). Meanwhile, HSRN-1 is mixed with naphtha from the cracking of heavier fractions in MIX-1 before being sent to HDT-1 to be desulfurized. HDT-1 produces hydrogen sulfide gas (H2S-1), liquefied petroleum gas (LPG-1), desulfurized naphtha (LSRN-2, HSRN-3, NAP-4) and fuel gas (FG-1). H2S-1 is sent to the Sulfur Recovery Unit (SRU) where Sulfur (S) is extracted and finally sold. All LPG (LPG-1-2-3) are sent to MIX-6 and subsequently to the LPG recovery unit (LPG), from which treated LPG (LPG-5) is sold. Similar to the ADU outputs, the desulfurized naphtha from HDT-1 can be classified as light (LSRN-2) and heavy (HSRN-3) or wild (NAP-4). HSRN-3 is sent to a mixer (MIX-4), possibly with purchased naphtha (PCHN-3-2) and/or naphtha from the hydrocracker (HCR-3). The output of MIX-4 (HSRN-5) is the feedstock for the Reformer (REF). FG-1 goes to the Fuel Gas Header (FGH), supplying fuel gas (FG-5) to the entire refinery. In the case that NAP-4 is produced from HDT-1, it is also mixed with purchased naphtha (PCHN-3-1) and/or naphtha from the hydrocracker (HCR-4) in MIX-5 whose output of NAP-5 is sent to the reformer. The products from the reformer are Hydrogen Gas (H2), Fuel Gas (FG-3), LPG (LPG-2) and reformate (REFs). H2 is a feed to the HDT while reformate is used as a gasoline blending component. FG-3 is sent to the FGH.

In the second case involving NAP-1 exiting ADU, the processing route is similar to the first case in that NAP-1 is mixed with naphtha from cracking processes in MIX-2 before being hydrotreated in HDT-2. The products from HDT-2 are H2S-2, LPG-3, desulfurized naphtha of LSRN-3, HSRN-4 and NAP-3 and FG-2. Each product has the exact same route as the products from HDT-1. Other than distillation, naphtha is also produced from the cracking of distillation bottoms in the Visbreaker (VIS), Coker (COK), Catalytic Cracker (FCC), Hydrocracker (HCR). VIS has the lowest severity while COK has the highest.

A few assumptions are taken into consideration in developing the superstructure:

- The intermediate products from the Visbreaker (VIS), delayed Coker (COK), Fluidized Catalytic Cracker (FCC) and Hydrocracker (HCR) are assumed to be heavy naphtha (that is, heavier fractions of naphtha)
- It is assumed that the API for medium and heavy crude oils is >33° whereas for light crude oil, the API is >33°

The processing of medium and heavy crude oils typically require more severe processes, hence COK, FCC and HCR are enforced as possible external sources of naphtha in such a case whereas VIS and FCC are the possible external naphtha sources for the processing of light crude oils which require less severe processing.

General formulation of logical constraints for process synthesis problems: Based on the depicted superstructure of processing alternatives for naphtha exiting the ADU in Fig. 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:

$$(z_{LSRN\text{-}1} \vee z_{LSRN\text{-}3}) \Leftrightarrow y_{MIX\text{-}3} \tag{1}$$

This is equivalent to the following two logic propositions:

$$\begin{gathered}(z_{LSRN\text{-}1} \vee z_{LSRN\text{-}3}) \Rightarrow y_{MIX\text{-}3}\\ y_{MIX\text{-}3} \Rightarrow (z_{LSRN\text{-}1} \vee z_{LSRN\text{-}3})\end{gathered} \tag{2}$$

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

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

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

Thus, we obtain the following algebraic constraints:

$$\begin{gathered}y_{MIX\text{-}3} \geq z_{LSRN\text{-}1}\\ y_{MIX\text{-}3} \geq z_{LSRN\text{-}3}\\ z_{LSRN\text{-}1} + z_{LSRN\text{-}3} \geq y_{MIX\text{-}3}\end{gathered} \tag{5}$$

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

Consider now the use of the logical relation exclusive or as given by the following:

$$(z_{LSRN\text{-}1} \veebar z_{LSRN\text{-}3}) \Leftrightarrow y_{MIX\text{-}3} \tag{6}$$

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

$$z_{LSRN\text{-}1} + z_{LSRN\text{-}3} = y_{MIX\text{-}3} \tag{7}$$

$$z_{LSRN\text{-}1} + z_{LSRN\text{-}3} = 1 \tag{8}$$

However, there are three possible pitfalls in the use of this logical relation which are all attributable to the logical constraint Eq. 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 Eq. 7 and 8 enforce that $y_{MIX\text{-}3} = 1$ 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 $(z_{LSRN\text{-}1}, z_{LSRN\text{-}3}, y_{MIX\text{-}3}) = (0, 0, 0)$ which is the hypothetical case of no crude oil feed is available.

Thus, the constraints given by Eq. 5 best enforce the design specification that MIX 3 is selected if and only if LSRN-1 or LSRN-3 is produced.

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:

$$\underset{k=1,2,\cdots,M}{\vee} Y_{u,k} \Leftrightarrow Y_u \;\; \forall u \in U = \{1, 2, \cdots, N\} \tag{9}$$

which is equivalent to:

$$\left(\underset{k=1,2,\cdots,M}{\vee} Y_{u,k} \Rightarrow Y_u\right) \wedge \left(Y_u \Rightarrow \underset{k=1,2,\cdots,M}{\vee} Y_{u,k}\right), \quad \forall u \in U \tag{10}$$

Transforming these logic propositions into inequalities yields:

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

$$\begin{aligned}
&Y_u \Rightarrow \underset{k=1,2,\cdots,M}{\vee} Y_{u,k} && \forall u \in U \\
&\neg Y_u \vee \left(\underset{k=1,2,\cdots,M}{\vee} Y_{u,k}\right) && \forall u \in U \\
&\left(1 - y_u\right) + \sum_{k=1}^{M} y_{u,k} \geq 1 && \forall u \in U \\
&\sum_{k=1}^{M} y_{u,k} - y_u \geq 0 && \forall u \in U
\end{aligned} \tag{12}$$

The MILP model formulation is summarized as follows:

$$\begin{aligned}
\min \quad & Z = \sum c_u + f(x) + d^T y \\
\text{s.t.} \quad & g_u(x) \leq 0 \\
& f_u \leq M_u y_u \\
& y_u - y_{u,k} \geq 0 \quad \forall i \in I, k = 1, 2, \ldots, M \\
& \sum_{k=1}^{M} y_{u,k} - y_u \geq 0 \quad \forall i \in I \\
& x \in \Re^n, y_u \in \{0,1\}, c_u \geq 0, c \in \Re^m
\end{aligned}$$

Logical constraints for processing alternatives of naphtha in refineries: 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. For simplicity, note that the abbreviations iff stands for if and only if and i-s stands for is/are selected. Parentheses are used to improve readability:

- ADU i-s iff (HDT-1 or HDT-2) I-s:

$$Y_{ADU} \Leftrightarrow (Y_{ADU\text{-}1} \underline{\vee} Y_{HDT\text{-}2})$$

- (HDT-1 or HDT-2) i-s iff SRU i-s:

$$(Z_{H2S\text{-}1} \vee Z_{H2S\text{-}2}) \Leftrightarrow Y_{SRU}$$

- (HSRN-3 or HSRN-4) i-s iff MIX-4 i-s:

$$(Z_{HSRN\text{-}3} \vee Z_{HSRN\text{-}4}) \Leftrightarrow Y_{MIX\text{-}4}$$

- (NAP-3 or NAP-4) i-s iff MIX-5 i-s:

$$(Z_{NAP\text{-}3} \vee Z_{NAP\text{-}4}) \Leftrightarrow Y_{MIX\text{-}5}$$

- (HDT-1 or HDT-2) i-s iff (MIX-3 and MIX-4), or (MIX-3 and MIX-5), or MIX-5 I-s:

$$\left(Y_{HDT-1} \vee Y_{HDT-2}\right) \Leftrightarrow \begin{pmatrix} \left(Y_{MIX-3} \wedge Y_{MIX-4}\right) \vee \left(Y_{MIX-3} \wedge Y_{MIX-5}\right) \\ \vee Y_{MIX-5} \end{pmatrix}$$

- (HSRN-5 or NAP-5) i-s iff REFu i-s:

$$(Z_{HSRN\text{-}5} \underline{\vee} Z_{NAP\text{-}5}) \Leftrightarrow Y_{REFu\text{-}5}$$

- (HDT-1 or HDT-2) i-s iff LPG i-s:

$$(Y_{HDT\text{-}1} \vee Y_{HDT\text{-}2}) \Leftrightarrow Y_{LPG}$$

- (FG-1 or FG-2 or FG-3 or FG-4) i-s iff FGH i-s:

$$(Z_{FG\text{-}1} \vee Z_{FG\text{-}2} \vee Z_{FG\text{-}3} \vee Z_{FG\text{-}4}) \Leftrightarrow Y_{FGH}$$

- ISO i-s iff HDT-1 i-s:

$$(Z_{ISO} \vee Z_{REF}) \Leftrightarrow Y_{BLND}$$

Generalized Disjunctive Programming (GDP) formulation: Generalized Disjunctive Programming (GDP), with Raman and Grossmann (1993, 1994) as its proponents, is an alternative modeling framework that has been found to be amenable in translating physical intuition into more formal mathematical expressions particularly in chemical-engineering-related problems, as it is more recently substantiated by Furman and Androulakis (2008). Since there will be conditional tasks or equipment that may be selected in the final refinery topology, the use of GDP is of particular interest, since process synthesis problems naturally lead to models where the solution space is disjoint and there is a strong logic on the connectivity among the different tasks (Raman and Grossmann, 1993, 1994).

To develop a GDP formulation, it is necessary to identify the conditional constraints from among those that must hold for all synthesis alternatives. The conditional constraints are represented with disjunctions and assigned a Boolean variable that represents its existence. Although disjunctions and logic propositions are useful in modeling design alternatives especially in chemical engineering applications, they cannot be included in conventional mathematical programming models (such as Mixed-Integer Programs (MIP)) without reformulations into logical constraints in algebraic equality of inequality forms. This is one of the reasons that calls for the adoption of GDP as it is able to handle disjunctions and logic propositions directly in which, design alternatives in terms of design and structural specifications can be formulated in the more intuitive representation of logic propositions while constraints with discrete variables are represented through disjunctions. Furthermore, the solution strategy of convex hull reformulation of GDP into mixed-integer programs avoids the use of big-M logical constraints which present weak relaxation, thus yielding a tighter linear programming relaxation (Turkay and Grossmann, 1996). The GDP formulation is summarized as follows:

$$\begin{aligned}
\text{min} \quad & Z = \sum c_u + f(x) + d^T y \\
\text{s.t.} \quad & g_u(x) \le 0 \\
& \begin{bmatrix} Y_i \\ h_i(x) \le 0 \\ c_i = \gamma_i \end{bmatrix} \vee \begin{bmatrix} \neg Y_i \\ B^i(x) = 0 \\ c_i = 0 \end{bmatrix} i \in D \\
& \Omega(Y) = \text{true} \\
& x \in \Re^n, y \in \{0,1\}^q, Y_i \in \{\text{true}, \text{false}\}^m, c_u \ge 0, c \in \Re^m
\end{aligned}$$

COMPUTATIONAL EXPERIENCE

Computational experiments and numerical studies on the proposed modeling approach within the mixed-integer optimization framework of MILP and GDP formulations for the flowsheet superstructure optimization problem considered in this study are coded and implemented using GAMS 22.8 modeling language platform. Two design scenarios as distinguished by the API gravity of the crude oil charge to the ADU are considered in the computational experiments conducted, namely for light crude oil mixture as characterized by API > 33° and heavy crude oil mixture as characterized by API = 33°. Both scenarios are developed based on conventional distillation column design and refinery economics, in which products from ADU are either: (1) separated into light straight run naphtha (LSRN-1) and heavy straight run naphtha (HSRN-1), or (2) separated in the form of an undifferentiated class of naphtha (NAP-1) typically termed as wild naphtha in the industry.

DISCUSSION OF COMPUTATIONAL RESULTS

The optimal refinery topology or configuration generated by the MILP and the GDP are, as expected, identical for both design scenarios. As depicted in Fig. 2 and 3, the optimal solutions of both models select an identical processing route comprising the same process units and material streams and their interconnections but at different processing levels. It is noteworthy that the optimal topology generated by each formulation agrees reasonably well with the topology of real-world existing refineries reported in standard references on the refining industry (Hydrocarbon Processing, 2008; Gary *et al*., 2007; Meyers, 2003; Maples, 2000). A closer inspection of Fig. 2 and 3 reveals that it is economically optimal to build a reformer and a hydrotreater within a single site based on the particular economics that is investigated in the numerical example.

The optimal objective function value of total investment cost which accounts for a summation of the fixed capital costs, variable operating costs and the raw material costs of purchasing the required crude oil slate, has been validated by comparing the values tabulated in Table 1 against industrial data available in the open literature. For instance, the annualized total investment

Table 1: Optimal objective function values

	Light crude oil processing		Heavy crude oil processing	
Model type	MILP	GDP	MILP	GDP
Optimal objective value (in million Malaysian ringgit per year)	2744	2465	2743	2453

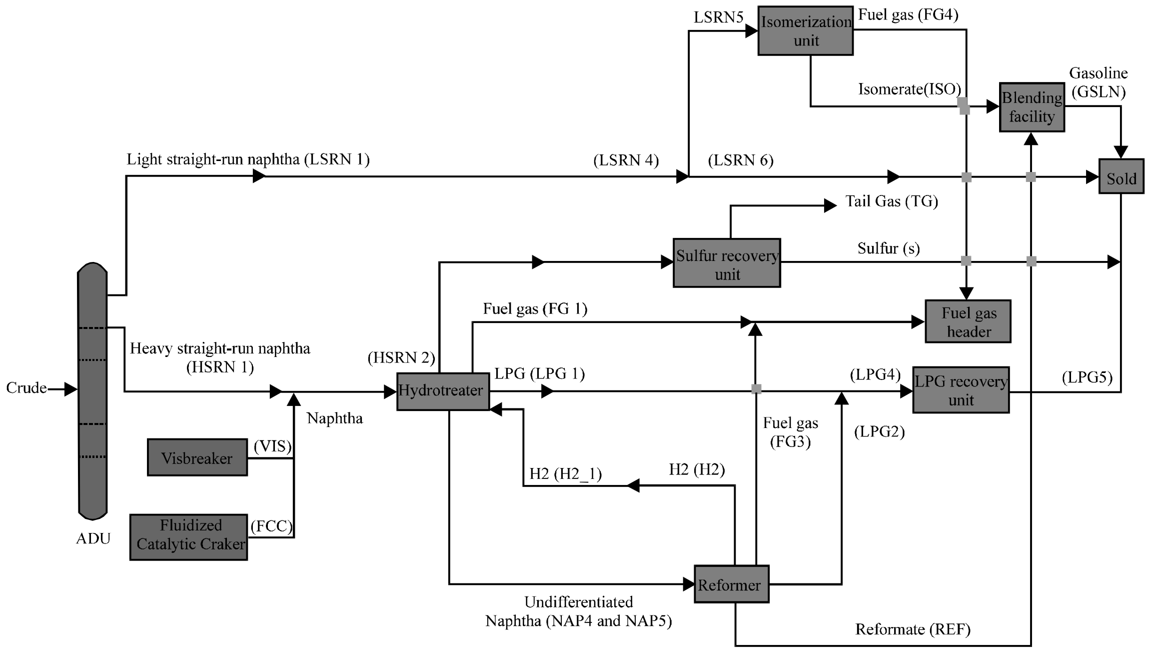

Fig. 2: Optimal refinery topology of the naphtha processing subsystem for light crude oil charge (API > 33°)

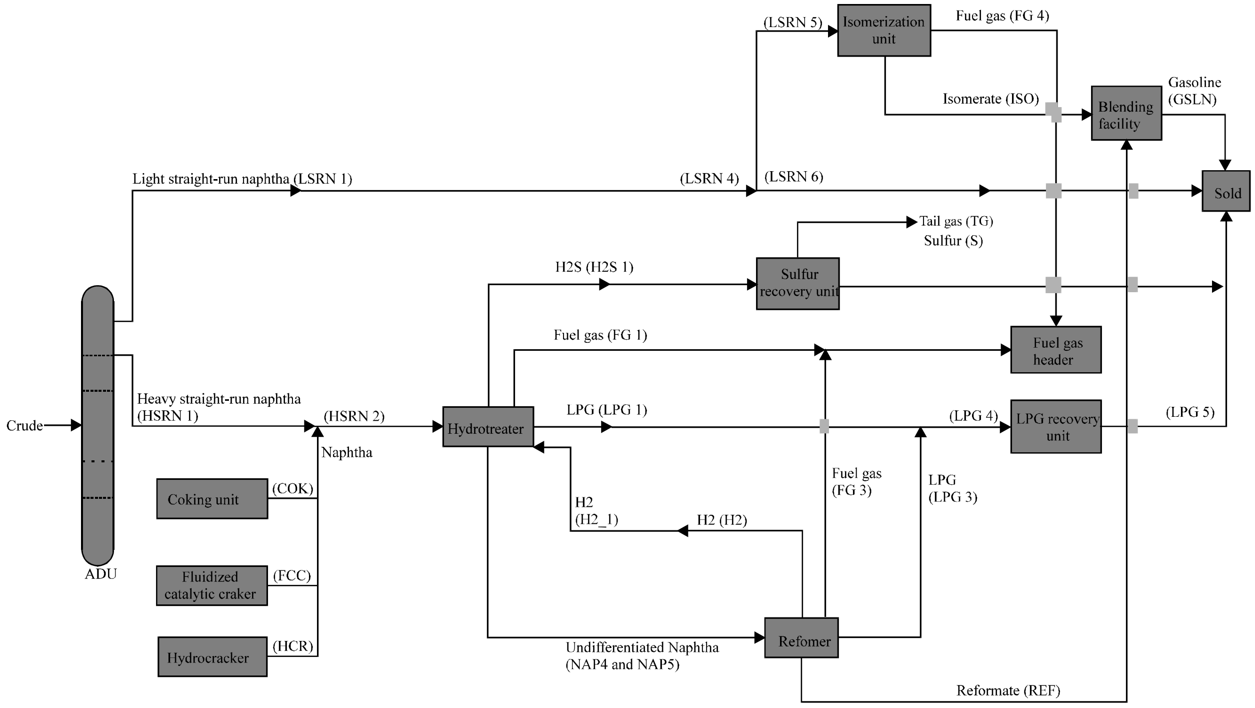

Fig. 3: Optimal refinery topology of the naphtha processing subsystem for heavy crude oil charge (API = 33°)

cost of the Bharat Petroleum Corporation Limited Refinery in Mahul, Bombay, India was estimated to be approximately RM2700 million which by inspection, is of relatively reasonable accuracy with our results (Hydrocarbon Processing, 2006). It is noteworthy that in this respect, the GDP model offers a more cost-effective solution by registering a lower total investment cost.

Table 2: Model sizes and computational statistics

Type of formulation	MILP	GDP
Solver	GAMS/CPLEX10	GAMS/LogMIP
No. of constraints	336	195
No. of continuous variables	77	95
No. of binary variables	80	22
No. of iterations	26	23
CPU time (sec)	Trivial (0.031)	Trivial (0.030)

The associated model sizes and computational statistics are reported in Table 2. As observed from the table, a GDP formulation typically offers a smaller model size relative to its MILP counterpart and hence, is likely to be more amenable for implementing extensions to this study that encompasses design features required for a more complex refinery.

In the final analysis, the strength of this study includes improved computational performance through incorporating engineering insights in process synthesis problems by using logical constraints on certain design and structural specifications. This is accomplished within a conventional MILP framework that presents the advantage of considering the effects of all relevant constraints simultaneously, thus affording a global perspective to the model. However, since the typical algorithm for MILP requires solving an LP subproblem at each node of the search tree, all the constraints must be linear equalities or inequalities. This imposes a restriction on the expressiveness of MILP as a modeling language as some problems may require a very large number of variables and constraints. Hence, this gives rise to our attempt to adopt the alternative modeling framework of GDP.

CONCLUSION

This study attempts to extend the existing optimization modeling strategies of integrating qualitative-based information in synthesis problems by using logical constraints. The novelty of the proposed approach lies in the application of logical constraints that enforce certain design specifications and structural specifications on the interconnectivity of the process units and materials streams in determining an optimal refinery topology. These logical constraints have been proven to be logic cuts that are algebraic linear inequalities or linear equalities that serve to reduce the computational time of an MILP or GDP by providing information that increases the efficiency of the enumeration procedure employed in the algorithms of the associated model solvers. In addition, this study also provides some insights on a generalized form of the logical constraints for synthesis and design problems and on how to identify possibly inconsistent integer constraints derived from logic propositions. On the overall, the proposed modeling approach offers a potential for assessing an optimal oil refinery topology via a discrete optimization approach.

ACKNOWLEDGMENT

The main author gratefully thanks Ali Elkamel for conceiving the initial ideas that have led to an extended study as in the present form and Aida Azwana Sabidi, the undergraduate research assistant in this study.

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