High Level Optimization Model for the Retrofit Planning of Process Networks

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To Professor Jim Douglas for his leadership and contributions in the area of process synthesis.

Abstract

The retrofit design of a network of processes over several time periods is addressed in this paper. A strategy is proposed that consists of a high level to analyze the entire network, and a low level to analyze a specific process flowsheet in detail. A methodology is presented for the high level to model process flowsheets and retrofit modifications using a multiperiod generalized disjunctive programming (GDP) model. This problem is reformulated as a mixed-integer linear program (MILP) using the convex hull formulation. Two examples that illustrate the proposed model are presented. The results show that the proposed GDP model provides a significant benefit over the existing network without retrofit, and provides a clear advantage over intuitively choosing modifications based on heuristics. To illustrate the performance benefits of using the convex hull formulation, the problem is also modeled as an MILP with big-M constraints.

Introduction

The area of process synthesis has mainly concentrated on integrating subsystems and flowsheets for the design of new processes, or "grassroots" design. Many algorithms and techniques have been developed to synthesize and optimize processes as different areas of process synthesis become better understood[14]. The less thoroughly explored area of retrofit synthesis, however, addresses one of the most prevalent problems in the chemical processing industry, which is the evaluation and redesign of existing plants. Processes can be retrofitted to achieve such goals as increasing throughput, reducing energy consumption, improving yields, and reducing waste generation. Retrofit designs may involve relatively small modifications (e.g. addition of equipment), or essentially tearing down the existing plant and replacing it by a new one. The retrofit problem is difficult due to the many constraints of a preexisting operation such as layout, available space, piping, and operating conditions. It is the goal of this work to address retrofit design of networks of chemical processes. This is a problem that has received little attention in the literature.

Work in retrofit design has been limited due to the difficulties described above and due to the many modification possibilities, which causes the problem to grow greatly in size. For instance, Grossmann *et al*.[15] show that for retrofit of a distillation sequence separating a mixture of N components, the number of tasks considered is $N - 1$ times that for the grassroots design.

The combinatorial nature of retrofit synthesis is the reason that research in the area to date has focused primarily on modifying a particular subsystem or equipment type. For a general review of retrofit issues see Grossmann *et al.*[15] As with the work in process synthesis, most literature for retrofit deals with Heat Exchanger Networks (HENs). Recent work on HENs retrofit includes procedures proposed by Kralj *et al.*[16] who use a stepwise simultaneous superstructural approach, Bochenek and Jezowski[4] who use an adaptive random search method, and Briones and Kokossis[5,6] who applied a mathematical programming and pinch analysis decomposition scheme and later used retrofit Hypertargets in a conceptual programming approach. Other subsystem work has been done by Papageorgaki and Reklaitis[20] and subsequently by Georgiadis *et al.*[12] who proposed optimal retrofit procedures for multi-purpose batch chemical plants. Seo *et al.*[23]

developed optimization techniques for the redesign of crude distillation columns. And Fraser and Hallale[10] proposed a method for the retrofit of mass exchange networks using the pinch technology that was developed for HENs.

Works that deal with retrofitting subsystems while also taking into account the retrofit of effected process networks include a method by Linhoff and Eastwood[17] that uses pinch technology for overall site optimization, and an approach by Zhang and Zhu[27] that uses simultaneous optimization of HENs and process changes.

Strategies to solve retrofit problems at the level of an individual flowsheet have been proposed by Grossmann *et al*.[15] who give a general outline for dealing with process retrofits, and by Fisher *et al*.[9], who present a systematic procedure for developing and screening retrofit opportunities. The method by Fisher *et al*., based on Douglas' hierarchy for design[8], is perhaps the most comprehensive to date, but is not systematic for predicting the retrofit changes. In spite of the work described above, there still exists no systematic strategy that unifies the retrofit design of all subsystems in an existing process or network of processes.

Companies in the chemical processing industry and related industries often have several site locations worldwide. Each of these sites may contain multiple processing plants which themselves may contain a series of different processes. These types of large-scale operations make the task of considering where to make retrofit improvements a difficult one. The application of an optimization model to this problem would be quite useful. However, the formulation of detailed models for each of the processes in a plant network is a cumbersome task involving the collection of many types of data. In fact, the data collection step alone may be too time consuming to make process modeling worthwhile. Therefore, we aim to provide a screening tool where the optimization model is formulated from a limited amount of process data.

The focus of this paper will be at the level of retrofitting a network consisting of several interconnected processes. A methodology is proposed that relies on a multiperiod generalized disjunctive programming (GDP) model that is reformulated as a mixed-integer linear program (MILP).

Problem Statement

The specific problem is as follows. An existing network of chemical processes is given, for which each process can possibly be retrofitted for improvements such as higher yield, increased capacity, and reduced energy consumption. Given limited capital investment to make process improvements and cost estimations over a specified time horizon, the problem consists of identifying those modifications that yield the highest economic improvement in terms of Economic Potential (EP) [8]. We define EP as the income from product sales minus the cost of raw materials, energy, and process modifications.

Methodology

We propose to address the retrofit problem using a hierarchical approach and mathematical programming tools. Unlike the hierarchy of five decision levels proposed by Douglas[8] for process synthesis, our method uses two levels: a high level for simultaneously analyzing the entire network, and a low level for analyzing a specific process flowsheet in detail. The focus of this paper is on the development of the high level model.

The nature of our retrofit problem requires the high level model to be fairly detailed in order to capture all the design and operation parameters most affected by process modifications. As an initial step, we assume that the high level model is linear. This is done to ease the computational effort in solving the large and complex proposed problem. Mass and energy balances are represented with linear equations, meaning that operating conditions are assumed to be fixed with constant temperatures and pressures for all process streams. Our aim is to model the proposed retrofit problem by developing a multi-period Generalized Disjunctive Programming (GDP) model that is reformulated into a multi-period MILP using convex hull transformations for each disjunction. This approach is in contrast to the use of conventional MILP formulations that rely on big-M constraints[25].

For the high level model, a linear programming (LP) model is developed from the process flowsheet using the procedure outlined below. An aggregated model is used to predict bounds for best process performance information independent of detailed design modifications. To construct the model for each process in the network (Figure 1) we proceed as follows:

1. Represent each flowsheet using only essential equipment, combining units when possible.
2. Set the operating conditions, fixing all stream temperatures and pressures.
3. Establish linear mass and energy balances that account for stoichiometry, yield, energy irreversibilities, etc.
4. Use balances in step 3 to formulate an LP model of the process that will determine all process flow rates.
5. Identify potential improvements and estimate the cost to implement them.

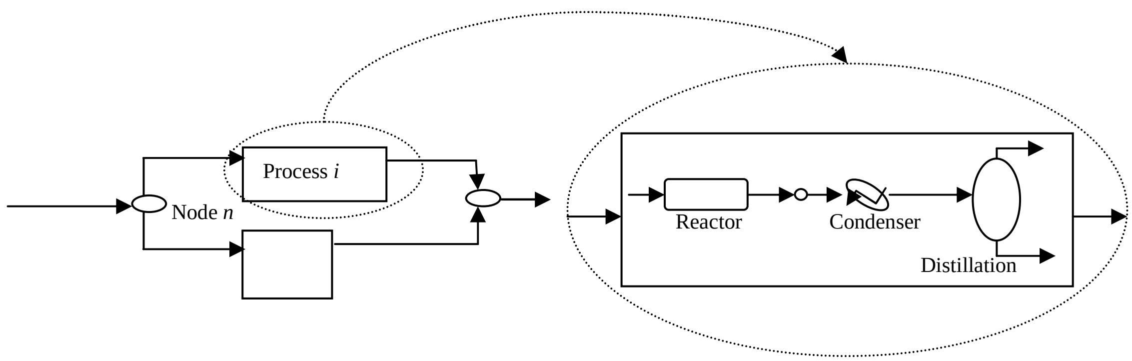

Figure 1. Sample Process Network and Process Flowsheet

It should be noted that the first four steps are described in detail in Biegler *et al*.[3]. Step 5 makes use of a variety of tools and techniques in process synthesis (e.g. pinch analysis[24], attainable region[2,13]). This step represents the major challenge in the proposed methodology. We assume in this paper that major modifications considered are typically for increasing production capacity and/or conversion, and for improving energy recovery.

High Level GDP Model

The proposed model is next set up to identify potential improvements that are to be realized through retrofit projects over T time periods and with limited capital in each of these periods. To model the modifications we will use Generalized Disjunctive

Programming[22], a logic-based representation of mixed integer problems where constraints associated with discrete variables are represented through disjunctions.

The objective function to be maximized is the economic potential over a planning horizon of T time periods. Costs for reactants, energy and modifications, and profits from product sales are included in the EP. Disjunctions are used to model changes in operating modes and design modifications. Operating modes $m \in M_i$ for each process i correspond to either existing operating conditions $\left(m_0 \in M_i\right)$, or to new conditions $\left(m \in M_i,\ m \neq m_0\right)$ that result from a retrofit project (e.g. higher yield, higher throughput, lower energy). The Boolean variables Y_{im}^t represent the selection of operating mode m for process i in each time period t, while W_{im}^t represents the decision to make design change m for process i in period t. Note that W_{im}^t can be regarded as the Boolean variable for project selection, while Y_{im}^t can be regarded as the Boolean variable that defines the operation as a function of the decisions W_{im}^t. M_i is the set of operating modes m for each process i, with the first element corresponding to no changes to the existing process i. The set of process balances that correspond to each operating mode m in each time period t can be written as:

$$A_{im}^t x_i^t \leq b_{im}^t \quad i \in P,\ m \in M_i,\ t = 1...T \tag{1}$$

The cost c_i^t for modifying process i in time period t is given by:

$$c_i^t = FC_{im}^t \quad i \in P,\ m \in M_i,\ t = 1...T \tag{2}$$

where FC_{im}^t is the fixed cost associated with design change m. LC^t specifies the limit on funds available to invest in retrofit projects in time period t. Funds not invested in a given time period do not accrue for use in subsequent time periods. The continuous variables x_i^t and x_n^t correspond to flow rates associated with process $i \in P$ at time t and node $n \in N$ (mixers and splitters) at time t, respectively. Chemical and energy prices are given by p^t. The GDP model (P1) with logic constraints is as follows:

(P1)

$$\max EP = \sum_{t \in T}\left[\left(p^t\right)^T x^t - \sum_{i \in P} c_i^t\right] \qquad (3)$$

s.t.

$$D_n x_n^t = d_n^t \qquad n \in N, \quad t = 1..T \qquad (4)$$

$$\bigvee_{m \in M_i}\begin{bmatrix} Y_{im}^t \\ A_{im}^t x_i^t \le b_{im}^t \end{bmatrix} \qquad i \in P, \quad t = 1...T \qquad (5)$$

$$\bigvee_{m \in M_i}\begin{bmatrix} W_{im}^t \\ c_i^t = FC_{im}^t \end{bmatrix} \qquad i \in P, \quad t = 1...T \qquad (6)$$

$$\sum_t w_{im}^t \le 1 \qquad i \in P, \quad m \in M_i \setminus m_0 \qquad (7)$$

$$\sum_{i \in P} c_i^t \le LC^t \qquad t = 1...T \qquad (8)$$

$$Y_{im}^t \rightarrow \left(\bigwedge_{\tau > t} Y_{im}^\tau\right) \qquad i \in P, \quad m \in M_i, \ t = 1...T \qquad (9)$$

$$\left(Y_{im}^t \bigwedge_{\tau < t}\left(\neg Y_{im}^\tau\right)\right) \rightarrow W_{im}^t \qquad i \in P, \quad m \in M_i, \ t = 1...T \qquad (10)$$

$$Y_{im}^t, W_{im}^t \in \{True, False\}$$

$$x^t, c_i^t \ge 0 \qquad x^t = \left\{x_i^t \cup x_n^t\right\}$$

The objective function (3), the Economic Potential, accounts for the income and expenses over the time periods $t \in T$. Equation (4) represents the mass balances over each node *n* that interconnects the processes. The first disjunction (5), which is an exclusive OR, selects the corresponding operating mode for the retrofit project *m* for each process *i* in each time period *t*. The second disjunction (6), which is an exclusive OR, selects the specific retrofit project *m*, including no changes $m_0 \in M_i$ that is to be implemented in a given time period *t*. Notice that for the case when no project m_0 is selected, $c_i^t = 0$. Equation (7) enforces a specific design change to be made in not more than one time period. In other words, once a modification is made for a given process, it cannot be made again in a subsequent time period. This constraint also ensures that investment costs for a given design change will be charged in the proper time period. Equation (8) limits the expenses for the retrofit projects. Equation (9) is a logic constraint stating that an operating mode Y_{im}^t selected in time period *t* implies that the same operating mode Y_{im}^τ will continue to be selected for subsequent time periods τ, where $\tau > t$. For example, if process *i* is modified to operate with increased capacity at time period 1, the larger capacity is also realized in time periods 2 and 3. Finally, the second logic constraint (10) sets the time period in which the design change *m* is made. This ensures that the cost for that change is charged in the proper time period.

MILP Reformulation

The convex hull formulation by Balas[1] is used to convert the GDP in (P1) into an MILP[22,25]. Consider the disjunction in (5),

$$\bigvee_{m \in M_i} \begin{bmatrix} Y_{im}^t \\ A_{im}^t x_i^t \le b_{im}^t \end{bmatrix} \quad i \in P, \quad t = 1...T \tag{11}$$

To obtain the convex hull of (11) the continuous variables are disaggregated, creating a variable for each disjunction (12).

$$x_i^t = \sum_{m \in M_i} x_{im}^t \qquad i \in P, \quad t = 1...T \tag{12}$$

$$0 \le x_{im}^t \le U_{im}^t y_{im}^t \qquad i \in P, \quad m \in M_i, \quad t = 1...T \tag{13}$$

$$A_{im}^t x_{im}^t \le b_{im}^t y_{im}^t \quad i \in P, \quad m \in M_i, \quad t = 1...T \tag{14}$$

$$\sum_{m \in M_i} y_{im}^t = 1 \quad i \in P, \ t = 1...T \tag{15}$$

Boolean variables are replaced by corresponding binary variables y_{im}^t. Variable bounds and modification equations are now rewritten in terms of the disaggregated and binary variables (see Equations (13) and (14)). Here U_{im}^t are appropriate upper bounds for the variables x_{im}^t. Since exactly one term of the disjunction must be true, Equation (15) enforces the requirement that only one binary variable be activated. Applying the convex hull to (6) yields the following constraints,

$$c_i^t = \sum_{m \in M_i} c_{im}^t \quad i \in P, \ t = 1...T \tag{16}$$

$$c_{im}^t = FC_{im}^t w_{im}^t \qquad i \in P, \quad m \in M_i, \quad t = 1...T \tag{17}$$

$$\sum_{m \in M_i} w_{im}^t = 1 \quad i \in P, \ t = 1...T \tag{18}$$

The reformulation also includes the integer forms of the logic constraints[22,26]. The reformulation along with the mixed-integer forms of the logical constraints in (P1) leads to the following MILP model:

(P2)

$$\max EP = \sum_{t \in T} \left[\left(p^t\right)^T x^t - \sum_{i \in P} c_i^t \right] \quad (19)$$

$$s.t.$$

$$D_n x_n^t = d_n^t \qquad n \in N, \quad t = 1 \ldots T \quad (20)$$

$$x_i^t = \sum_{m \in M_i} x_{im}^t \qquad i \in P, \quad t = 1 \ldots T \quad (21)$$

$$c_i^t = \sum_{m \in M_i} c_{im}^t \qquad i \in P, \quad t = 1 \ldots T \quad (22)$$

$$A_{im}^t x_{im}^t \le b_{im}^t y_{im}^t \quad i \in P, \quad m \in M_i, \quad t = 1 \ldots T \quad (23)$$

$$x_{im}^t \le U_{im}^t y_{im}^t \quad i \in P, \quad m \in M_i, \quad t = 1 \ldots T \quad (24)$$

$$c_{im}^t = FC_{im}^t w_{im}^t \quad i \in P, \quad m \in M_i, \quad t = 1 \ldots T \quad (25)$$

$$c_{im}^t \le U_{im}^t w_{im}^t \quad i \in P, \quad m \in M_i, \quad t = 1 \ldots T \quad (26)$$

$$\sum_{m \in M_i} \mathrm{y}_{\mathrm{im}}^{\mathrm{t}} = 1 \qquad i \in P, \quad t = 1 \ldots T \quad (27)$$

$$\sum_{m \in M_i} \mathrm{w}_{\mathrm{im}}^{\mathrm{t}} = 1 \qquad i \in P, \quad t = 1 \ldots T \quad (28)$$

$$\sum_t w_{im}^t \le 1 \qquad i \in P, \quad m \in M_i \setminus m_0 \quad (29)$$

$$y_{im}^t \le y_{im}^\tau \qquad i \in P, \quad m \in M_i, \quad \forall \tau > t = 1 \ldots T \quad (30)$$

$$y_{im}^t \le \sum_{\tau < t} y_{im}^\tau + w_{im}^t \quad i \in P, \quad m \in M_i, \quad t = 1 \ldots T \quad (31)$$

$$\sum_{i \in P} c_i^t \le LC^t \qquad t = 1 \ldots T \quad (32)$$

$$x^t, c_i^t, x_{im}^t, c_{im}^t \ge 0 \qquad x^t = \left\{ x_i^t \cup x_n^t \right\}$$

$$y_{im}^t, w_{im}^t \in \{0,1\}$$

In the above problem the objective function (19) and node balances (20) are identical to equations (3) and (4) in (P1), respectively. x_{im}^t are the disaggregated variables for the disjunctions in (5) which have the associated binary variables y_{im}^t; c_{im}^t are the disaggregated costs for the disjunctions in (6) which have the associated binary variables w_{im}^t. Note that the inequalities in (5) and the costs in (6) are written in terms of disaggregated variables and corresponding 0-1 variables. Also, variable upper bounds are specified for x_{im}^t and c_{im}^t to assure they take a value zero when the corresponding term in the disjunction is not selected.

It should be noted that problem (P1) could also be reformulated as an MILP with big-M constraints. As with the convex hull formulation, the Boolean variables are replaced by the corresponding binary variables. A big-M parameter is introduced on the right hand side of the process constraint so that the inequality is rendered redundant if $y_{im}^t = 0$ $\left(\text{or } w_{im}^t = 0\right)$. If $y_{im}^t = 1$ $\left(\text{or } w_{im}^t = 1\right)$, the inequality is enforced. The binary variables y_{im}^t and w_{im}^t are summed over the set of modifications so that only one operating mode and design decision can take place, respectively. Additionally, the binary variable w_{im}^t is summed over the set *T* so that only one design decision can take place per time period (see Equation (7)). As applied to disjunctions (5) and (6) in problem (P1), the big-M constraints yield:

(P2a)

$$
\begin{aligned}
& A_{im}^t x_i^t \le b_{im}^t + BM_{im}\left(1 - y_{im}^t\right) \quad i \in P,\ m \in M_i,\ t = 1...T \\
& \sum_{m \in M_i} y_{im}^t = 1 \quad i \in P,\ t = 1..T \\
& c_i^t = FC_{im}^t w_{im}^t \quad i \in P,\ m \in M_i,\ t = 1...T \\
& \sum_{m \in M_i} \mathrm{w}_{\mathrm{im}}^{\mathrm{t}} = 1 \quad i \in P,\ \ t = 1...T \\
& \sum_{t=1}^{T} w_{im}^t \le 1 \quad i \in P,\ m \in M_i
\end{aligned}
$$

The remaining constraints are converted to MILP form exactly as in the convex hull case so that the rest of the model is identical to (P2). The Big-M reformulation leads to smaller problem sizes because it does not require the disaggregation of variables as in the convex hull formulation. However, even carefully selected choices for big-M parameters may yield poor LP relaxations[25].

Ranking of Projects

The proposed MILP model (P2) can easily be extended to handle cases where it is necessary to rank the potential value of each of the proposed retrofit modifications. Specifically, by applying appropriate constraints, the model can be used as a screening tool to choose which single project would be the most promising. The following constraint specifies that only a single modification decision can be made in the process network across the time horizon,

$$\sum_{t=1}^{T} \sum_{i \in P} \sum_{m \in M_i} w_{im}^t = 1 \tag{33}$$

Similar screening restrictions can be made to determine the best modification for each process, or for each time period as shown in (34) and (35), respectively.

$$\sum_{t=1}^{T} \sum_{m \in M_i} w_{im}^t = 1 \ \forall i \tag{34}$$

$$\sum_{i \in P} \sum_{m \in M_i} w_{im}^t = 1 \quad t = 1 \ldots T \tag{35}$$

Modifications are ranked from most profitable to least profitable by rerunning the model with an iterative procedure. The integer cuts for the model in iteration K are generated from the optimal solution of the model solved in the previous iteration K - 1. For the case of the overall ranking of projects with the equation in (32), the integer cuts IC^K that make infeasible the choice of the binary from subsequent iterations is as follows:

$$IC^K = \left\{ \sum_{(i,m,t) \in B^K} w_{im}^t - \sum_{(i,m,t) \in N^K} w_{im}^t \le \left| B^K \right| - 1 \right\} \tag{36}$$

where $B^K = \{(i,m,t) | \ w_{im}^t = 1\}$, and $N^K = \{(i,m,t) | \ w_{im}^t = 0\}$.

Process Network Model

For convenience in the presentation, models (P1) and (P2) have been presented in generic form. In this section we provide the specific equations that apply to the process network. Network modifications could include any or all of the following changes for each process: increase in conversion, increase in capacity, or no modification. A site-wide modification for energy is also possible. To formulate the GDP model representation for these modifications, we define the variables f to denote material and energy flow rates in the network. Also, we consider the following basic linear equations:

$$f_i^{Prod,t} = \eta_{im} f_i^{R,t} \tag{37}$$

$$f_i^{Prod,t} \le CAP_{im} \quad (38)$$

$$R_k^t - R_{k-1}^t - Q_S^t + Q_W^t = \sum_{hot} Q_{hot,k}^t - \sum_{cold} Q_{cold,k}^t \qquad k = 1 \ldots K \quad (39)$$

Equation (37) represents the mass balance in terms of the conversion η_{im}, while the inequality in (38) specifies the capacity limits CAP_{im} for each process. Equation (39) represents the transshipment energy equations where Q_S^t and Q_W^t are the steam and cooling water requirements, R_k^t is the residual heat of each interval *k*, and $Q_{hot,k}^t$ and $Q_{cold,k}^t$ are the hot and cold streams of interval *k*[3,19]. Incorporating the above equations into (P1) yields the following GDP model (see nomenclature section at end of paper):

(P3)

$$\max EP = \sum_{t\in T}\left[\left(p^t\right)^T f^t - \sum_{i\in P} c_i^t - ec^t\right] \quad (40)$$

$s.t.$

$$D_n f_n^t = d_n^t \qquad n \in N \quad t = 1...T \quad (41)$$

$$f_i^t \geq DEM_i^t \qquad i \in P \quad t = 1...T \quad (42)$$

$$\underset{m\in M_i}{\vee}\begin{bmatrix} Y_{im}^t \\ f_i^{Prod,t} = \eta_{im} f_i^{R,t} \\ f_i^{Prod,t} \leq CAP_{im} \end{bmatrix} \qquad i \in P \quad t=1...T \quad (43)$$

$$\underset{m\in M_i}{\vee}\begin{bmatrix} W_{im}^t \\ c_i^t = FC_{im}^t \end{bmatrix} \qquad i \in P \quad t=1...T \quad (44)$$

$$\begin{bmatrix} X_0^t \\ Q_S^t = \sum_k \sum_{cold} Q_{cold,k}^t \\ Q_W^t = \sum_k \sum_{hot} Q_{hot,k}^t \end{bmatrix} \vee \begin{bmatrix} X_1^t \\ R_k^t - R_{k-1}^t - Q_S^t + Q_W^t = \sum_{hot} Q_{hot,k}^t - \sum_{cold} Q_{cold,k}^t \\ \mathrm{k} = 1...\mathrm{K} \end{bmatrix} \quad t = 1...T \quad (45)$$

$$\underset{\mathrm{mod}}{\vee}\begin{bmatrix} V_{\mathrm{mod}}^t \\ ec^t = EFC_{\mathrm{mod}}^t \end{bmatrix} \qquad \mathrm{mod} \in MOD, \quad t = 1...T \quad (46)$$

$$\sum_{i\in P}\left(c_i^t\right) + ec^t \leq LC^t \qquad t = 1...T \quad (47)$$

$$Y_{im}^t \rightarrow \left(\underset{\tau>t}{\wedge} Y_{im}^\tau\right), \qquad i \in P, \quad m \in M_i, \ t = 1...T \quad (48)$$

$$\left(Y_{im}^t \underset{\tau<t}{\wedge}\left(\neg Y_{im}^\tau\right)\right) \rightarrow W_{im}^t, \qquad i \in P, \quad m \in M_i, \ t = 1...T \quad (49)$$

$$\sum_t w_{im}^t \leq 1 \qquad i \in P, \quad m \in M_i \setminus m_0 \quad (50)$$

$$X_{\mathrm{mod}}^t \rightarrow \left(\underset{\tau>t}{\wedge} X_{\mathrm{mod}}^\tau\right) \qquad \mathrm{mod} \in MOD, \ t = 1...T \quad (51)$$

$$\left(X_{\mathrm{mod}}^t \underset{\tau<t}{\wedge}\left(\neg X_{\mathrm{mod}}^\tau\right)\right) \rightarrow V_{\mathrm{mod}}^t \qquad \mathrm{mod} \in MOD, \ t = 1...T \quad (52)$$

$$\sum_t v_1^t \leq 1 \qquad i \in P, \quad m \in M_i \setminus m_0 \quad (53)$$

$$\mathrm{Y}_{\mathrm{im}}^t, W_{im}^t, X_{\mathrm{mod}}^t, V_{\mathrm{mod}}^t \in \{True, False\}$$

$$f^t, c_i^t \geq 0 \qquad f^t = \left\{f_n^t \cup f_i^t\right\} \qquad f_i^t = \left\{f_i^{Prod,t} \cup f_i^{R,t}\right\}$$

The objective function (40) for the Economic Potential includes profits from sales as well as capital costs c_i^t and energy costs ec^t over the time periods $t \in T$. Equation (41) represents the mass balances over each node *n* that interconnects the processes, while equation (42) ensures that the demand DEM_i^t is met for each product *Prod*. The first disjunction (43) selects one of the corresponding operating modes for the retrofit project *m* for each process *i* in each time period *t*, where projects *m* include modifying process conversion, capacity, or both. The second disjunction (44) selects one of the specific retrofit projects *m*, including no changes $m_0 \in M_i$ where modification costs are set to zero ($c_i^t = 0$). The next disjunction (45) selects the appropriate operating mode so that X_0^t corresponds to no energy integration and X_1^t enforces the transshipment equations. Using the Boolean variable V_{mod}^t, the last disjunction (46) selects the specific retrofit project *mod*, including no changes $\mathrm{mod}_0 \in MOD_i$ where energy modification costs are set to zero ($ec_i^t = 0$). Equations (50) and (53) enforce a specific design change to be made in only one time period for conversion/capacity and energy, respectively. Equation (47) limits the expenses for the retrofit projects. Equations (48) and (51) are logic constraints that select the operating mode in process *i* in the time periods τ following the change to that mode in a previous time period *t*. Finally, the remaining logic constraints (49) and (52) set the time period in which the design changes *m* and *mod* are made, respectively.

By modifying the definition of modes *m* for the retrofit projects, an alternate representation of the disjunctions in (P3) can be developed (see Appendix). However, this second representation includes bilinear expressions which effectively give rise to a nonconvex optimization problem that requires global techniques for its solution. Due to this complication we have elected to use the first form for representing disjunctions.

Numerical Examples

To illustrate our proposed approach we consider the following two examples. The first example involves a simple three-process network. The second example deals with a 5-process, 8-chemical superstructure for the manufacture of acetaldehyde, acrylonitrile, cumene, phenol, and acetone.

The GDP (P3) is reformulated into an MILP as shown in (P2). Both examples were solved on a 500 MHz Pentium III PC, with 256 MB RAM. The models were coded in the GAMS modeling environment[7] and solved with CPLEX 7.0.

Example 1: Three-Process Network

The retrofit is considered of a plant making products *D* and *E* from raw materials *A*, *B*, and *C* (Figure 2). We use a 1-year planning horizon of 3 time periods consisting of 4 months. Modifications for increased conversion and capacity only are considered with specifications given in Table 1. Data on the fixed costs associated with each modification along with the available investment capital is shown in Table 2. These fixed costs include investment costs for all new/modified equipment in the process associated with the specified changes. Purchase and sale prices for the raw materials and products are given in Table 3. Black-box (input/output) models are used for each process. The maximum amounts of raw materials A, B, and C available are 550, 36 and 333 tons/day, respectively. The demands for products D and E are 233 and 210 tons/day, respectively.

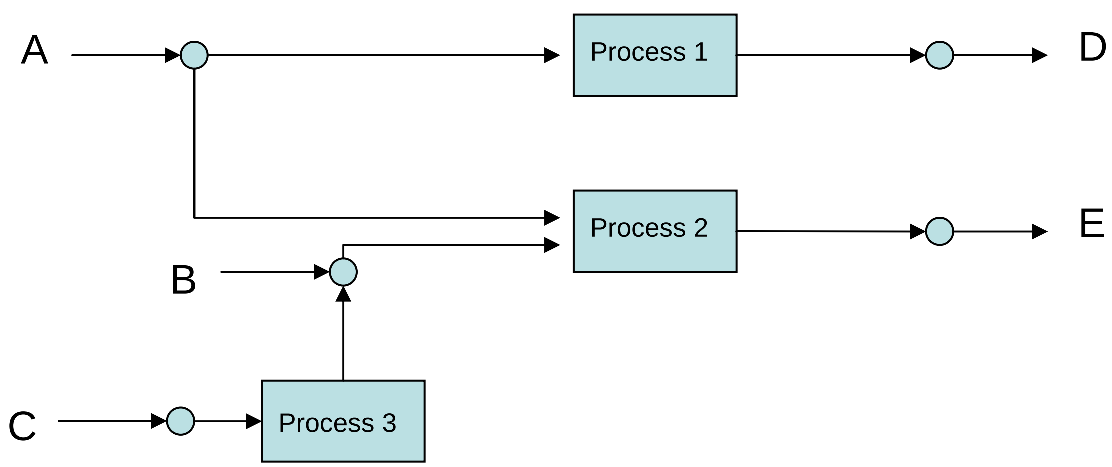

Figure 2. Process Network for Example 1

Table 1. Process Retrofits for Each Process in Example 1

Process	**Conversion**	*Conversion Retrofit*	*Capacity (tons/day)*	*Capacity Retrofit (tons/day)*
1	0.9	0.95	175	233
2	0.85	0.9	210	350
3	0.8	0.85	107	250

Table 2. Fixed Costs and Capital Limits for Each Time Period in Example 1

Time Period	**Fixed Cost Conversion ($)**	*Fixed Cost Capacity ($)*	*Fixed Cost Conversion & Capacity ($)*	*Capital Limit ($)*
1	100,000	350,000	450,000	200,000
2	75,000	225,000	300,000	250,000
3	60,000	250,000	310,000	350,000

Table 3. Market Prices for Process Components in Example 1

Component	A	B	C	D	E
Price ($/ton)	70	336	216	454	308

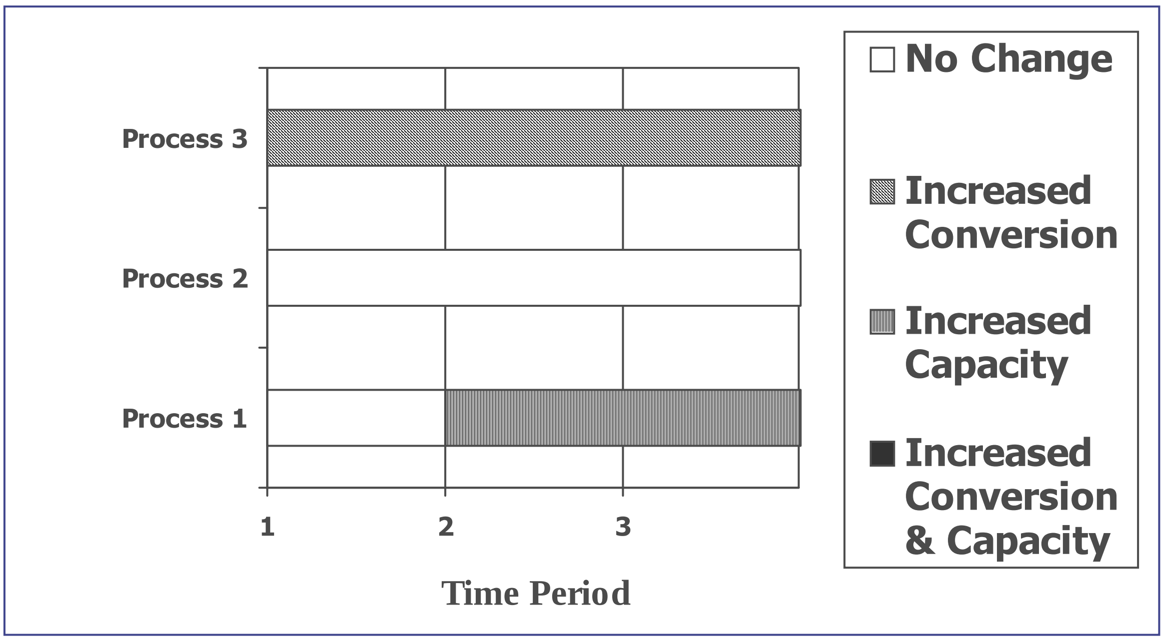

Figure 3. Process Retrofits over Time Horizon for Example 1

The convex hull MILP formulation corresponding to (P2) has 394 constraints, 244 continuous variables, and 36 discrete variables. The optimal solution is an EP of $11,841,130 obtained in 0.731 CPUs after 82 simplex iterations. This integer solution was obtained at the root node, and hence no branching was required. Investment in time periods 1, 2, and 3 is $100,000, $225,000 and $0, respectively. The predicted modifications are shown in Figure 3. Note that process 1 was modified for increased capacity in time period 2, process 2 was not modified, and process 3 was modified for increased conversion in time period 3.

The problem was also modeled using conventional big-M constraints to reformulate the GDP into an MILP to show the benefits of the convex hull formulation. This MILP is more compact with 328 constraints, 124 continuous variables and 36 discrete variables. The big-M model gives the same solution, but takes longer to solve the problem to optimality; 1.81 CPUs after 2526 simplex iterations branching on 388 nodes. The explanation for this performance was the weaker upper bound of the LP relaxation ($113,716,667 versus $12,815,897 for convex hull).

Example 2: Five-Process Network

The process network shown in Figure 4 is a modification of an example from Iyer and Grossmann[11]. Aggregated models representing each process were developed and integrated into a network superstructure as described earlier in the paper. We do not include explicit data for this problem due to its size; however this information is available from the authors upon request.

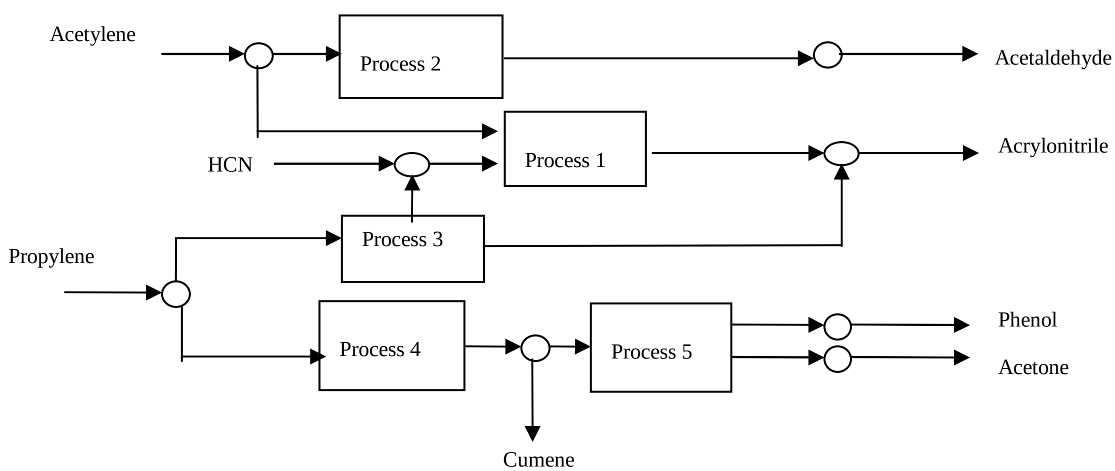

Figure 4. Example: Five Process Network

The convex hull MILP formulation (P2) has 2171 constraints, 1690 continuous variables, and 66 discrete variables. The optimal solution is an EP of $180.1 million obtained in 1.04 CPUs after 854 simplex iterations branching on 4 nodes. One reason for the good computational performance is the tight upper bound of the profit of $184.9

million from the relaxed LP. The investment per time period is shown in Table 4. The energy modification for the entire site was selected in time period 1, and the other process modification selections are summarized in Figure 5. Note that process 1 was modified for increased capacity in time period 1, process 2 undergoes no modification, process 3 was modified for increased conversion and capacity in time period 2, process 4 was modified for increased conversion and capacity in time period 3, and process 5 was modified for increased capacity in time period 1.

Table 4. Investment for Modifications in Each Time Period for Example 2

Time Period	1	2	3
Investment ($)	221,000	220,000	$210,000

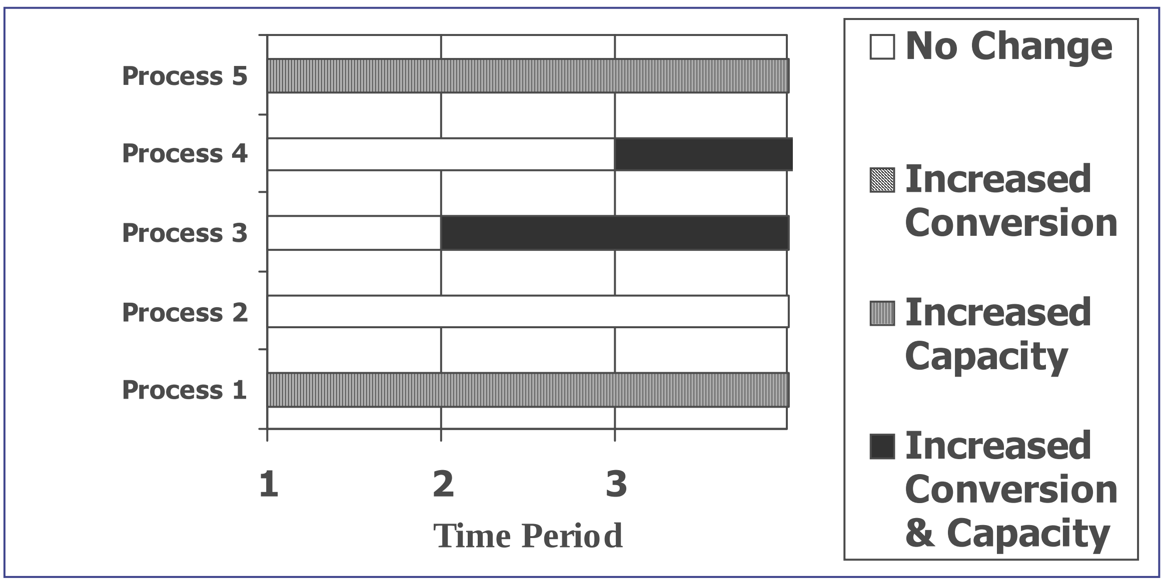

Figure 5. Process Retrofits over Time Horizon for Example 2

The solution when no modifications are allowed gives an EP of $76.4 million. This is 46% less than the EP obtained by the model presented in this work. The solution to the model where modifications are chosen intuitively based on a heuristic that sequentially selects the project with the largest process improvement per period is shown in Figure 6. In time period 1, process 1 was modified for increased conversion and capacity, in time period 2, process 5 was also modified for increased conversion and capacity, and in time period 3, process 2 was modified for increased capacity. An EP of $158.6 million was obtained, which is $22 million less (or 12% less) than the EP obtained with the proposed model. This shows the value of the optimization approach outlined in this paper.

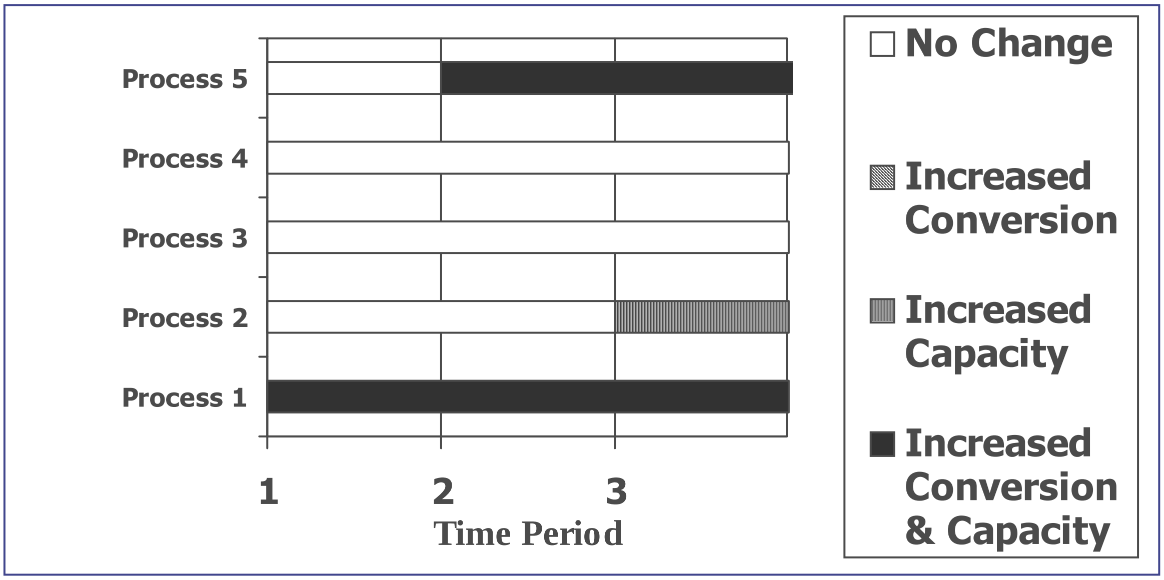

Figure 6. Process Retrofits over Time Horizon using Heuristic

The problem was also modeled using conventional big-M constraints to reformulate the GDP model into an MILP. The big-M model, whose parameters were carefully selected to yield a valid and tight upper bound, gives the same solution, but takes longer to converge; 19.91 CPUs after over 19,010 iterations branching on 2686 nodes. The relaxed solution of the big-M model has an EP of $748 million, as compared to the relaxed solution of $184.9 million from our model. The large gap between the relaxed and optimal solutions for the big-M case causes the longer solution times of the big-M model as compared to the model with the convex hull formulation. For larger examples with bigger process models and more modification options, longer solution times can be expected.

Model for Ranking Projects

The extension of the proposed model to rank the projects based on their economic potential was applied to Example 2. The model for screening retrofit projects contains

2150 constraints, 1690 continuous variables, and 66 discrete variables. Every iteration took approximately 1.5 CPUs to run. The model is first solved to rank the top five projects in all the processes over the entire time horizon. The solution results are shown in Table 5.

Table 5. Screening Model for Example 2 with Top Ten Ranking Retrofit Projects

Rank	**Economic Potential (million-$)**	**Retrofit Project**	**Time Period Implemented**
1	158.485	Capacity Increase in Process 1	1
2	158.482	Conversion/Capacity Increase in Process 1	1
3	131.107	Capacity Increase in Process 1	2
4	131.105	Conversion/Capacity Increase in Process 1	2
5	108.664	Conversion/Capacity Increase in Process 3	1

The screening model was then run for the case where projects are ranked by time period. Table 6 describes what modifications had the most potential in each time period. Note that these projects coincide with the ones predicted by the simultaneous solution in Figure 5.

Table 6. Screening Model for Example 2 with Top Project in Each Time Period

Time Period	**Retrofit Project**
1	Capacity Increase in Process 1
2	Conversion/Capacity Increase in Process 3
3	Conversion/Capacity Increase in Process 4

Conclusion

A high level MILP model has been proposed to address the retrofit design of process networks. The proposed model allows for multiple types of modifications in each time period. Examples were given that illustrate the robustness of the Generalized Disjunctive Programming approach with convex hull reformulation. The convex hull formulation gives a tight LP relaxation which leads to faster solution times when compared to the big-M constraints. Extensions of the model were presented that include methods to screen and rank modification alternatives.

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Nomenclature

BM_{im} = big-M parameters for process *i* for operating mode *m*

c_i^t = cost for modifying process *i* in time period *t*

CAP_{im} = capacity limits for process *i* in operating mode *m*

DEM_i^t = production requirement in process *i* in period *t*

ec^t = energy costs in time period *t*

EP = economic potential which is revenue minus costs

$f_i^{Prod,t}$ = material and energy flow rates for component *Prod* in process *i* in period *t*

FC_{im}^t = fixed cost associated with design change *m* in process *i* in period *t*

LC^t = available funds to invest in retrofit projects in time period *t*

M_i = set of operating modes/design changes *m* for each process *i*

N = set of nodes *n* that represent mixers and splitters

p^t = chemical and energy prices in time period *t*

P = set of processes *i*

$Q_{cold,k}^t$ = cold stream in interval *k* of heat exchanger in period *t*

$Q_{hot,k}^t$ = hot stream in interval *k* of heat exchanger in period *t*

Q_S^t = heat exchanger steam requirement in period *t*

Q_W^t = heat exchanger cooling water requirement in period *t*

R_k^t = residual heat in interval *k* of heat exchanger in period *t*

U_{im}^t = upper bounds for the process flow rates x_{im}^t

V_{mod}^t = represents the decision to make energy integration design change *mod* in period *t*

W_{im}^{t} = represents the decision to make design change *m* for process *i* in period *t*

x_i^t = flow rates for process *i* in time period *t*

x_{im}^t = flow rates for process *i* for operating mode *m* in time period *t*

x_n^t = flow rates for node *n* in time period *t*

X_{mod}^{t} = represents the selection of energy integration mode *mod* in each period *t*

Y_{im}^t = represents the selection of operating mode *m* for process *i* in each time period *t*

η_{im} = conversion fraction for reaction in process *i* in operating mode *m*

References

(1) Balas E. Disjunctive Programming and a Hierarchy of Relaxations for Discrete Optimization Problems. *SIAM J. Alg. Disc. Meth.*, **1985**, 6, 466.

(2) Balakrishna S.; Biegler, L. T. A Constructive Targeting Approach for the Synthesis of Isothermal Reactor Networks. *Ind. Eng. Chem. Res.*, **1992**, 31, 300.

(3) Biegler L. T.; Grossmann, I. E.; Westerberg,A.W. *Systematic Methods of Chemical Process Design*. Prentice Hall: Upper Saddle River, NJ, 1997.

(4) Bochenek R.; Jezowski, J. Adaptive Random Search Approach for Retrofitting Flexible Heat Exchanger Networks. *Hungarian Journal of Industrial Chemistry*, **1999**, 27(2), 89-97.

(5) Briones V.; Kokossis, A. Hypertargets: A Conceptual Programming Approach for the Optimisation of Industrial Heat Exchanger Networks – II. Retrofit Design. *Chemical Engineering Science*, **1999**, 54, 541-561.

(6) Briones V.; Kokossis, A. New Approach for the Optimal Retrofit of Heat Exchanger Networks. *Computers & Chemical Engineering*, **1996**, 20(suppl A), S43-S48.

(7) Brooke A.; Kendrick, D.; Meeraus, A. *GAMS: A User's Guide* Scientific Press: Palo Alto, CA, 1992.

(8) Douglas J. M. *Conceptual Design of Chemical Processes.* McGraw-Hill: New York, 1987.

(9) Fisher W. R.; Doherty, M. F.; Douglas, J. M. Screening of Process Retrofit Alternatives. *Industrial & Engineering Chemical Research*, **1987**, 26, 2195.

(10) Fraser D. M.; Hallale, N. Retrofit of Mass Exchange Networks Using Pinch Technology. *AIChE Journal*, **2000**, 46(10), 2112-2117.

(11) Iyer R. R.; Grossmann, I. E. A Bilevel Decomposition Algorithm for Long-Range Planning of Process Networks. *Industrial & Engineering Chemical Research*, **1998**, 37(2), 474.

(12) Georgiadis M. C.; Rotstein, G. E.; Macchietto, S. Optimal Layout Design in Multipurpose Batch Plants. *Industrial & Engineering Chemistry Research*, **1997**, 36(11), 4852-4863.

(13) Glasser, D.; Crowe, C.; Hildebrandt, D. A geometric approach to steady flow reactors: The attainable region and optimization in concentration space. *Ind. Eng. Chem. Res.*, **1987**, 26 (9), 1803.

(14) Grossmann I. E.; Cabellero, J.; Yeomans, H. Advances in Mathematical Programming for Automated Design, Integration and Operation of Chemical Processes. **1999**, Proceedings of the International Conference on Process Integration (PI'99), Copenhagen, Denmark.

(15) Grossmann I. E.; Westerberg, A. W.; Biegler, L. T. Retrofit Design of Processes. Proceedings of Foundations of Computer Aided Operations (Eds. G.V. Reklaitis and H.D. Spriggs), Elsevier, p.403 (1987).

(16) Kralj A. K.; Glavic, P.; Kravanja, Z. Retrofit of Complex and Energy Intensive Processes II: Stepwise Simultaneous Superstructural Approach. *Computers & Chemical Engineering*, **2000**, *24(1)*, 125-138.

(17) Linnhoff B.; Eastwood, A. R. Overall Site Optimization by Pinch Technology. *Chemical Engineering Research & Design*, **1997**, 75(suppl), S138-S144.

(18) McCormick, G. P. Computability of global solutions to factorable nonconvex programs – Part I – Convex underestimating problems. *Mathematical Programming*, **1976**, *10*, 147-175.

(19) Papoulias S. A.; Grossmann, I. E. A Structural Optimization Approach to Process Synthesis-II. Heat Recovery Networks. *Comp. Chem. Eng.*, **1983**, 7, 707.

(20) Papageorgaki S.; Reklaitis, G. V. Retrofitting a General Multipurpose Batch Chemical Plant. *Industrial & Engineering Chemistry*, **1993**, 32(2), 345-362.

(21) Quesada, I.; Grossmann, I. E. Global optimization of bilinear process networks with multicomponent flows. *Computers & Chemical Engineering*, **1995**, *12*, 1219-1242.

(22) Raman R.; Grossmann, I. E. Modeling and Computational Techniques for Logic Based Integer Programming. *Comp. Chem. Eng.*, **1994**, 18, 563.

(23) Seo J. W.; Kim, S. J.; Kim, K. H.; Oh, M.; Lee, T. H. Optimal Design of a Crude Distillation Column Using Optimization Techniques. *American Society of Mechanical Engineers, Pressure Vessels and Piping Division*, **1998**, 177-182.

(24) Tjoe T. N.; Linhoff, B. Using Pinch Technology for Process Retrofit. *Chem. Eng.*, **1986**, 93(8), 47.

(25) Turkay M.; Grossmann, I. E. Disjunctive Programming Techniques for the Optimization of Process Systems with Discontinuous Investment Costs-Multiple Size Regions. *Ind. Eng. Chem. Res.*, **1996**, 35(8), 2611.

(26) Williams H. P., *Model Building in Mathematical Programming, 2nd Edition,* Wiley: New York, 1985.

(27) Zhang J.; Zhu, X. X. Simultaneous Optimization Approach for Heat Exchanger Network Retrofit with Process Changes. *Industrial & Engineering Chemical Research*, **2000**, 4963-4973.

Appendix: *Modified Disjunction Representation*

By modifying the definition of modes m for the retrofit projects, an alternate representation of the disjunctions can be developed. In model (P1) a disjunctive term in (6) exists involving terms for every individual project as well as every combined modification. Consider as an example two possible modifications: M_1 to increase the yield from η^0 to η^{new}, M_2 to increase the capacity from CAP^0 to CAP^{new}. In model (P1) the corresponding disjunction would be as follows:

$$\begin{bmatrix} M_0 \\ f^{Prod} = \eta^0 f^R \\ f^{Prod} \le CAP^0 \end{bmatrix} \vee \begin{bmatrix} M_1 \\ f^{Prod} = \eta^{new} f^R \\ f^{Prod} \le CAP^0 \end{bmatrix} \vee \begin{bmatrix} M_2 \\ f^{Prod} = \eta^0 f^R \\ f^{Prod} \le CAP^{new} \end{bmatrix} \vee \begin{bmatrix} M_3 \\ f^{Prod} = \eta^{new} f^R \\ f^{Prod} \le CAP^{new} \end{bmatrix} \quad \text{(a)}$$

Note that in the above M_0 corresponds to the case with no changes, while M_3 corresponds to the case when both changes are applied. While the disjunction has four terms, the advantage is that the linearity of the yield and capacity constraints is retained.

To see why nonlinearities are introduced in the alternate representation, consider writing the following disjunctions and constraints:

$$\begin{bmatrix} M_1 \\ \eta = \eta^{new} \end{bmatrix} \vee \begin{bmatrix} \neg M_1 \\ \eta = \eta^0 \end{bmatrix} \qquad \text{(b)}$$

$$\begin{bmatrix} M_2 \\ CAP = CAP^{new} \end{bmatrix} \vee \begin{bmatrix} \neg M_2 \\ CAP = CAP^0 \end{bmatrix} \qquad \text{(c)}$$

$$f^{Prod} = \eta \ f^{R} \qquad \text{(d)}$$

$$f^{Prod} \leq CAP \qquad \text{(e)}$$

The first two disjunctions indicate whether or not a given modification is selected. Note that while equations (b), (c) and (e) are linear, equation (d) contains a bilinear expression. Convex underestimators can be used to convert these constraints types of constraints to linear form[18,21]. However, this effectively gives rise to a nonconvex optimization problem that requires global techniques for its solution.