Mixed-integer nonlinear programming models for optimal design of reliable chemical plants¹

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Abstract

Motivated by reliability/availability concerns in chemical plants, this paper proposes MINLP models to determine the optimal selection of parallel units considering the trade-off between availability and cost. Assuming an underlying serial structure for availability, we consider first a case where the system transitions between available and unavailable states, and second the case with an intermediate state at half capacity. Two non-convex MINLP models maximizing net profit are introduced for the two cases. In addition, a bi-criterion MINLP model is proposed to maximize availability and to minimize cost for the first case. It is shown that the corresponding epsilon-constrained model, where the availability is maximized subject to parametrically varying upper bound of the cost, can be reformulated as a convex MINLP. Availability is also incorporated in the superstructure optimization of process flowsheets. The performances of the proposed models are illustrated with a methanol synthesis and a toluene hydrodealkylation process.

Keywords: Reliability, Availability, Design, MINLP, Parallel units, Serial structure

1. Introduction

Plant availability has been a critical consideration for the design and operation of chemical processes, for it represents the expected fraction of normal operating time, which impacts directly the ability of meeting demands. Currently, discrete event simulation tools are used to evaluate reliability/availability of selected alternatives to simulate the behavior of every asset in a plant using historical maintenance data and statistical models (Sharda and Bury, 2008). However, this approach does not systematically consider all the alternatives as it would be the case in an optimization approach.

The goal of evaluating and optimizing reliability/availability quantitatively for various kinds of engineering systems and plants, has led to the development of the area of reliability

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¹This article is dedicated to the memory of Chris Floudas, a leader and pioneer of optimization and process systems engineering

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engineering, whose aim is to rationally consider the ability of a system to function properly. According to Zio (2009), major questions that are addressed include how to measure and evaluate system reliability, to detect the causes and consequences of system failures, strategies of system maintenance, and reliability-based design optimization (RBDO), which is relevant to the work in this paper.

One of the major challenges is the complexity of the system, which is the result of multistate behaviors that occur frequently in production plants, and topological complexities primarily faced by distributed service systems such as communication and transportation networks. Lisnianski et al. (2010) provide a comprehensive introduction to the study of multi-state system behaviors. Specifically, it addresses the use of Markov chain theory on both statistical and analytical methods. Petri-net based models have been widely used for the performance analysis of computer systems (Malhotra and Trivedi, 1995). Bayesian network is another accepted tool for the analysis of failure propagation in complex networks (Weber et al., 2012).

Compared with the other major research aspects in reliability engineering, reliabilitybased design optimization (RBDO) arises at the early stages for determining the topology and parameters of a system. Kuo and Prasad (2000) give an comprehensive review of this area. Aside from continuous parameter selections, discrete decisions regarding parallel redundancies are an important part of RBDO. Various types of methods have been used to obtain the optimal or suboptimal configurations, such as genetic algorithms (Coit and Smith, 1996), Monte Carlo simulation (Marseguerra et al., 2005) and heuristics (Hikita et al., 1992).

Research has also been done in chemical engineering to quantitatively analyze the reliability of the chemical plants. Rudd (1962) discusses the estimation of system reliability with parallel redundancies. Henley and Gandhi (1975) suggest using a minimal path method to evaluate failure propagation and the sensitivity of system reliability to unit reliability. Van Rijn (1987) provides a systematic overview of reliability, availability and maintenance and their industrial applications. (Thomaidis and Pistikopoulos, 1994, 1995) integrate flexibility and reliability in process design, but does not consider the possibility of having standby units in order to improve the availability of a system. Pistikopoulos et al. (2001) and Goel et al. (2003b) formulate an MILP model for the selection of units with different reliability and the corresponding production and maintenance planning for a fixed system configuration. Aguilar et al. (2008) address the reliability issue in utility plant design and operation by considering some pre-specified alternatives for redundancy, and for which they formulate and MILP model considering a limited number of failure scenarios. Terrazas-Moreno et al. (2010) formulate an MILP model using Markov chains to optimize the expected stochastic flexibility of an integrated production site by the selection of pre-specified alternative plants and the design of intermediate storage. Lin et al. (2012) model a simple utility system using Markov chain and carry out RAM (reliability, availability & maintainability) analysis iteratively to decide the optimal reliability design.

However, it is fair to state that, while a number of mixed-integer optimization models have been proposed to address various aspects of reliability, there are virtually no general rigorous mixed-integer programming models are specifically aimed at systematically selecting the type and number of parallel units for the optimal design of reliable chemical processes. In response to this gap, this work proposes a general optimization model to select parallel units in order to maximize availability and to minimize cost in serial systems, providing basic model properties.

In section 2, a motivating example is introduced, followed by problem statement in section 3 and nomenclature in section 4. In section 5, two non-convex MINLP models maximizing net profit are presented with/without intermediate states, respectively. In addition, considering maximizing availability and minimizing cost separately, a non-convex ϵ -constraint MINLP model is formulated that can be convexified for the basic case. Illustrative examples for these models are presented in section 6, along with applications to process synthesis problem.

2. Motivating example

To better focus on the parallel unit selection problem, we consider an air separation unit (ASU) shown in Figure 1 as a motivating example. Air is fed to a compressor followed by the after-cooler, and then the pre-purifier to remove impurities. After that, air is cooled by the gas product of nitrogen and liquid product of oxygen. Further refrigeration is provided by expansion through a turbine before entering the cold box.



Figure 1: Typical flowsheet of air separation units

The failure of any one of the operations can result in the failure of the entire system, which will prevent it from producing liquid and gas products, and hence satisfying customer demands. To increase the system availability, design alternatives are proposed for some operation stages. The availability superstructure is formulated as a serial system of sequential stages shown in the block diagram of Figure 2.

For example, we can choose to install one full-capacity unit for main air compression, whose failure will lead to system failure. Or it can have two half-capacity units instead, in which case the system maintains 50 percent of designed capacity when one of the two units fails. However, the second option might be more expensive.



Figure 2: The diagram of ASU reliability design alternatives. Each block represents a parallel unit with certain rate of capacity shown in the block

3. Problem statement

With the motivating example in mind, we define a general modeling framework for production systems with underlying serial structures for availability evaluation (Figure 3). Our goal is to determine design decisions regarding which potential parallel units to install, in order to maximize the system availability (i.e. probability that the system performs without failures), and hence sales revenue, while minimizing the total cost of the system.



Figure 3: A serial system

Before presenting detailed mathematical representations, we will describe in this section the basic logic followed by the two cases being investigated.

One of them is the basic case where all the stages need only one unit to work properly. A set of potential units $j \in J_k$ for each stage k are given with:

- Availabilities, i.e. the probability of each unit being available.
- Operating priorities (indicated by j), which means that a unit can only become active when all installed units that have higher priorities have failed.
- Cost rates, including installation and repair.

Based on the parameters provided above, the relationship between the availability of stage k and the selection of parallel units is established. The processing stages are divided into two kinds:

- Stages where potential parallel units are identical $(k \in K_{iden})$.
- Stages where potential parallel units have the same capacities, but are distinct in terms of availability or cost $(k \in K_{non})$.

In addition to the basic case, another type of design alternatives is applied. For example, the second design alternatives of the main air compression in the motivating example (see Figure 2) is to have two half capacity compressors, such that when one of them is failed, there is still half of the original output left. System availability is also redefined to capture the new behavior when having partial capacity.

4. Nomenclature

Indices

- k Stage
- j Parallel unit, smaller j has priority over larger j
- l Dummy variable for j

Sets

- K_{iden} Set of stages with identical parallel units
- K_{non} Set of stages with non-identical parallel units (K_{iden} and K_{non} is a partition of K)
- J_k Set of parallel units for each state

Parameters

n_k	Number of potential parallel units in stage k
p_k^i	Availability of single units in stage k with identical parallel units
$p_{k,i}^n$	Availability of single unit j in stage k with non-identical parallel units
c^{i} _inst_k	Investment for single units in stage k with identical parallel units
$c^i _repa_k$	Repair cost for single units in stage k with identical parallel units
$c^n_inst_{k,j}$	Investment for single unit j in stage k with non-identical parallel units
$c^n repa_{k,j}$	Repair cost for single unit j in stage k with non-identical parallel units
\overline{cost}	Upper bound of total cost
rv	Revenue rate of final product
pn	Penalty rate for not meeting lower bound of availability
bn	Bonus rate for exceeding upper bound of availability
A_lo	The lower bound of system availability arranged in the contract
$A_{-}up$	The upper bound of system availability arranged in the contract

Variables

Binary variable that indicates whether unit j of stage k is selected
Availability of stage k
Expectancy of units being repaired of stage k
Total repair cost for single units in stage k
Total cost for stage k
Total cost of system
Expected revenue
Expected penalty
Expected bonus
Net profit
Binary variable that indicate which one of the ranges A falls in
Components of A for corresponding range
Components of PN for corresponding components of A
Components of BN for corresponding components of A

5. Model Formulation

5.1. Binary state model

As mentioned in section 3, we will first consider the basic case where the system has only two states and introduce the corresponding MINLP model (SO).

Constraint (1) requires that for each stage k at least one unit j should be installed.

$$\sum_{j=1}^{n_k} y_{k,j} \ge 1, \quad k \in K \tag{1}$$

Constraint (2) is a symmetry breaking constraint for stages $k \in K_{iden}$, which requires that a unit can only be selected if the one with higher priority is selected.

$$y_{k,j+1} \le y_{k,j}, \quad k \in K_{iden}, j \in J_k \tag{2}$$

The availability of a stage depends on the number of installed parallel units and the corresponding availabilities. Considering the fact that the redundancies for one stage are usually no more than a few, we enumerate all possible cases for each stage to evaluate the availability.



Figure 4: Sample diagrams for single stages

Consider the diagram in Figure 4(a) as an example, where all the units are identical. If we introduce symmetry breaking constraints (2), unit j in stage k being selected means that all the potential units with higher priorities are selected. Considering all design alternatives, i.e. installing unit 1, installing unit 1 and 2 or installing unit 1, 2 and 3, there are 3 possible cases that the stage is functioning: Unit 1 is active; Unit 2 is active while unit 1 has failed; Unit 3 is active while unit 1 and 2 have failed. It is obvious that whether a case happens depends only on the existence of the unit that is active in it, and the probability for a possible case to take place depends on the availabilities of that particular unit and all the potential units with higher priorities. Thus, we have the following linear constraints:

$$P_1 = p_1 y_{1,1} + (1 - p_1) p_1 y_{1,2} + (1 - p_1)^2 p_1 y_{1,3}$$

which can be easily generalized to equation (3).

$$P_k = p_k \sum_{j=1}^{n_k} y_{k,j} (1 - p_k)^{j-1}, \quad k \in K_{iden}$$
(3)

The diagram in Figure 4(b) represents a stage $k \in K_{non}$ with non-identical parallel units, which are not restricted by symmetry breaking constraints. Hence, we cannot avoid nonlinearity by enumerating all the cases where the system is available as it was done for identical standby stages, which contributes to increasing the complexity of the analysis. The availability is represented by substracting the probabilities of unavailable cases (Goel et al., 2003a).

$$P_{k} = 1 - \prod_{j \in J_{k}} (1 - p_{k,j} y_{k,j}), \quad k \in K_{non}$$
(4)

For example, for the stage shown in Figure 4(b), we have

$$P_1 = 1 - (1 - p_{1,1}y_{1,1})(1 - p_{1,2}y_{1,2})(1 - p_{1,3}y_{1,3})$$

Notice that multi-linear terms of 0-1 variables are introduced, which will be linearized as shown in the next section. Based on equations (3) and (4), the availability of the system consisting of stages $k \in K$ is given by equation (5)

$$A = \prod_{k \in K} P_k \tag{5}$$

The total cost of each stage is the summation of investment and repair costs.

$$C_k = (c^i inst_k + c^i repa_k) \sum_{j=1}^{n_k} y_{k,j}, \quad k \in K_{iden}$$

$$\tag{6}$$

$$C_{k} = \sum_{j=1}^{n_{k}} y_{k,j} (c^{n} inst_{k,j} + c^{n} repa_{k,j}), \quad k \in K_{non}$$
⁽⁷⁾

The total cost of the entire system is then given by equation (8)

$$C^{tot} = \sum_{k \in K} C_k \tag{8}$$

5.1.1. Profit maximization

A typical way availability impacts the net profit is considered below, where system availability is reflected in revenue, penalty and bonus, and net profit is the summation of the three terms minus the summation of total costs.

$$max \quad NP = RV - PN + BN - C^{tot} \tag{9}$$

The total revenue is proportional to the availability of the system.

$$RV = rvA \tag{10}$$

Since RV is positive and maximized in the objective function (9), equation (10) can be

relaxed as follows.

$$RV \le rvA$$
 (11)

which can be combined with (5) and converted to (12):

$$lnRV - \sum_{k \in K} lnP_k \le lnrv \tag{12}$$

Since lnRV is concave separable, and $-\sum_{k\in K} lnP_k$ is convex, replacing (10) with (12) improves the quality of the convex underestimations for the spatial branch and bound search for global optimization.

Generally, in the contract between the plant and the customer, two reference bounds are set for the availability of the plant. As shown in Figure (5), if the actual availability of the plant does not meet the lower bound, the plant that provides products for the customer will be charged a penalty proportional to the difference. On the other hand, if the actual availability exceeds the upper bound, the customer will reward the plant with bonus that is also proportional to the difference.



The penalty and bonus are described by equation (13) and disjunction (14).

$$W_1 \stackrel{\vee}{=} W_2 \stackrel{\vee}{=} W_3 \tag{13}$$

$$\begin{pmatrix} W_1 \\ A \leq A . lo \\ PN = (A . lo - A)pn \\ BN = 0 \end{pmatrix} \lor \begin{pmatrix} W_2 \\ A . lo \leq A \leq A . up \\ PN = 0 \\ BN = 0 \end{pmatrix} \lor \begin{pmatrix} W_3 \\ A \geq A . up \\ PN = 0 \\ BN = (A - A . up)bn \end{pmatrix}$$
(14)

The convex-hull reformulation (Balas, 1985) of (14) yields (15) - (26), where w_1, w_2 and

 w_3 are binary variables for boolean variables W_1, W_2 and W_3 .

$$A = A^1 + A^2 + A^3 \tag{15}$$

$$PN = PN^{1} + PN^{2} + PN^{3} \tag{16}$$

$$BN = BN^1 + BN^2 + BN^3 (17)$$

$$A^1 \le w_1 A_lo \tag{18}$$

$$w_2 A_{-lo} \le A^2 \le w_2 A_{-up} \tag{19}$$

$$A^3 \le w_3 A_{-} u p \tag{20}$$

$$PN^1 = (A_low_1 - A^1)pn \tag{21}$$

$$PN^2 = 0 \tag{22}$$

$$PN^3 = 0 \tag{23}$$

$$BN^1 = 0 (24)$$

$$BN^2 = 0 \tag{25}$$

$$BN^3 = (A^3 - A_{-}upw_3)bn \tag{26}$$

Constraints (16), (17) and (21)-(26) can be reduced to (27) and (28)

$$PN = (A_{-}low_1 - A^1)pn \tag{27}$$

$$BN = (A^3 - A_{-}upw_3)bn \tag{28}$$

Thus, the linear equations (inequalities) (13), (15), (18)–(20) and (27)–(28) define the convex hull of (13) and (14).

In summary, the single objective MINLP (SO) maximizes net profit (9) subject to (1)-(8), (12), (13), (15), (18)-(20) and (27)-(28). This is a non-convex MINLP due to the nonconvexity of (5), which is involved in the objective (9).

5.1.2. Bi-criterion optimization and convexified formulation

Instead of maximizing net profit, we now consider problem (P1) that maximizes system availability (29) and minimizes total cost (30) subject to constraints (1)-(8), which has the interesting property that it can be reformulated as a convex MINLP problem.

 $\max A$ (29)

(30)

 $\min C^{tot}$

The bi-criterion optimization problem (P1)((1)-(8) and (29)-(30)) is solved through reformulation to the ϵ -constraint optimization problem (P1')((1)-(8), (29) and (31)), which maximizes system availability (29) subject to the upper bound of total cost as shown in equation (31). The upper bound of total cost is varied parametrically to generate a Paretooptimal curve.

$$C^{tot} \le \overline{cost} \tag{31}$$

As mentioned before, equation (4) for nonidentical units in (P1) involves multi-linear terms, and so does the objective function of (P1'), which causes the problem to be nonlinear and non-convex. In problem (P1'L), which is to be described in this section, we propose to linearize constraint (4) and convexify the objective function. In order to do so, the products over linear terms in (4) are expanded as summations over multi-linear terms, which are then linearized. Since in (4), the multiplication is done over the set J_k , we first propose the following new sets and parameters to enumerate the subsets of J_k . Set:

 $S_{k,m}$ Subset m of J_k

 \mathbb{S}_k The power set of J_k : $\mathbb{S}_k = \{S | S \subseteq J_k\}$

For example, if there are 3 potential units in stage 1 $(J_1 = \{1, 2, 3\})$, then the number of subsets in the power set S_1 is $2^3 = 8$, $S_1 = \{\emptyset, \{1\}, \{2\}, \{1, 2\}, \{3\}, \{1, 3\}, \{2, 3\}, \{1, 2, 3\}\}$.

The binary parameter $\alpha_{j,S}$ is defined to indicate whether unit j belongs to subset $S_{k,m}$: $\alpha_{j,k,m} = 1$ means that unit j belongs to subset $S_{k,m}$. Again, consider $J_1 = \{1, 2, 3\}$ as an example, then for $S_{1,4} = \{1, 2\}$, $\alpha_{1,1,4} = 1$, $\alpha_{2,1,4} = 1$, $\alpha_{3,1,4} = 0$. Table 1 gives a comprehensive example to show how $\alpha_{j,k,m}$ is defined for each alternative.

Table 1: An example of the corresponding relationship between $S_{k,m}$ and $\alpha_{j,k,m}$ in stage k

$\alpha_{j,k,m}$							
		j					
m	1	2	3				
1	0	0	0				
2	1	0	0				
3	0	1	0				
4	1	1	0				
5	0	0	1				
6	1	0	1				
7	0	1	1				
8	1	1	1				

To guarantee that all and only subsets of J_k are included in S_k , without any repetition or omission, we use the following equation to generate the subsets.

$$\alpha_{j,k,m} = \lfloor \frac{mod(m-1,2^j)}{2^{j-1}} \rfloor, \quad k \in K_{non}$$

We can consider $\alpha_{j,k,m}$ as the digit on the *j*th place of the binary form of m-1. The

following binary variables are then defined based on the above definition of S:

$$z_{k,m} = \prod_{j \in S_{k,m}} y_{k,j}, \quad k \in K_{non}, S_{k,m} \in \mathbb{S}_k$$

The following logic conditions hold for $z_{k,m}$ (Glover and Woolsey, 1974),

$$z_{k,m} \Leftrightarrow \Big(\bigwedge_{j \in S_{k,m}} y_{k,j}\Big), \quad k \in K_{non}, S_{k,m} \in \mathbb{S}_k, S \neq \emptyset$$
$$z_{k,m} = 1, \quad k \in K_{non}, S_{k,m} = \emptyset$$

which can be reformulated as the following linear inequalities (Raman and Grossmann, 1991),

$$z_{k,m} \le y_{k,j}, \quad k \in K_{non}, j \in S_{k,m}, S_{k,m} \in \mathbb{S}_k, S_{k,m} \ne \emptyset$$
(32)

$$z_{k,m} \ge \sum_{j \in S_{k,m}} y_{k,j} - |S_{k,m}| + 1, \quad k \in K_{non}, S_{k,m} \in \mathbb{S}_k$$
(33)

Based on the above definitions of the subsets $S_{k,m}$, the power set \mathbb{S}_k and the variable $z_{k,m}$, equation(4) is then reformulated as the following linear equations:

$$P_{k} = 1 - \prod_{j \in J_{k}} (1 - p_{k,j}y_{k,j}), \quad k \in K_{non}$$

$$= 1 - \sum_{S_{k,m} \in \mathbb{S}_{k}} (\prod_{j \in S_{k,m}} (-p_{k,j}y_{k,j})) (\prod_{j \in J_{k} \setminus S_{k,m}} 1), \quad k \in K_{non}$$

$$= 1 - \sum_{S_{k,m} \in \mathbb{S}_{k}} (\prod_{j \in S_{k,m}} (y_{k,j})) (\prod_{j \in S_{k,m}} -p_{k,j}), \quad k \in K_{non}$$

$$= 1 - \sum_{S_{k,m} \in \mathbb{S}_{k}} z_{k,m} \prod_{j \in S_{k,m}} (-p_{k,j}), \quad k \in K_{non}$$
(34)

As an example, the diagram shown in Figure 4(b) that has 3 distinct parallel units yields

$$P_{1} = 1 - (z_{1,1} + z_{1,2}(-p_{1,1}) + z_{1,3}(-p_{1,2}) + z_{1,4}(-p_{1,1})(-p_{1,2}) + z_{1,5}(-p_{1,3}) + z_{1,6}(-p_{1,1})(-p_{1,3}) + z_{1,7}(-p_{1,2})(-p_{1,3}) + z_{1,8}(-p_{1,1})(-p_{1,2})(-p_{1,3}))$$

Thus, the equations $P_k, k \in K$ are linear in model (P1L). On the other hand, let

$$A' = lnA = ln(\prod_{k \in K} P_k) = \sum_{k \in K} lnP_k$$
(35)

Since logarithmic functions are monotone, maximizing A' is equal to maximizing A. The

original objective function (29) can thus be replaced by (36).

$$maxA' = \sum_{k \in K} lnP_k \tag{36}$$

Since each term in the above summation is concave, A' is concave. Maximizing the concave function is equivalent to minimizing a convex function. Thus, the reformulated problem (P1'L) ((1)-(3), (5)-(8) and (31)-(36)) is a convex MINLP (i.e. the relaxed NLP of (P1'L) is convex).

5.2. Multi-state model

The models presented in the previous sections are based on the assumption that all of the stages as well as the entire system transitions between binary states, on and off, which means that for each single stage to be available, the fewest number of available units is 1. However, in practice, there is another strategy for increasing availability that is equally used as the simple back-up strategy considered previously. It is to let a few units (usually 2) share the workload. For example, in the typical case we consider in model (TS), in addition to the full capacity back-up pattern, some stages can have two units that both work at half of the designed capacity, and if one of them fails, the system can still operate at half capacity). The objective of model (TS) is to maximize the net profit based on the contracts production described in section 5.1.1.

For the augmented case, we define the following new indices, variables and parameters.

l,m	Aliases of j
$cp_{k,j}$	Capacity level of unit j in stage k
$y_{k,j}^F$	Binary variable representing the existence of the j th candidate unit in full
	capacity group of stage k
$y_{k,j}^H$	Binary variable representing the existence of the j th candidate unit in half
	capacity group of stage k
P_k^F	Probability of stage $k \in K$ working in full capacity
P_k^H	Probability of stage $k \in K$ working in half capacity
A^F	Probability of the whole system working in full capacity
A^H	Probability of the whole system working in half capacity

As shown in Figure 6, stage k may have two groups of potential units with full capacities and half capacities, respectively. Like what was done for the basic case in section 5.1, these units are numbered by index j in the order of operation priorities. It is also obvious that full capacity units, if they exist, will always have higher priorities than half capacity units.



For the stage to have enough capacity in normal conditions, we have constraint (37).

$$\sum_{j \in J_k^F} cp_{k,j} y_{k,j}^F + \sum_{j \in J_k^H} cp_{k,j} y_{k,j}^H \ge 1, \quad k \in K$$
(37)

The probability of stage k having half capacity is calculated in equation (38). $\prod_{j \in J_k^F} (1 - p_{k,j}^F y_{k,j}^F)$ is the probability that all full capacity units are failed, which is the premise of having half capacity. It reduces to 1 when full capacity units are not installed and $y_{k,j}^F = 0$. Then we calculate the conditional probability that only one unit j from the half-capacity group is left available, by enumerating all possible cases based on the available unit j. The expression means that, in the case where j is the only available unit, all potential units with higher operational priorities are failed (if selected), and all potential units with lower operational priorities are not selected.

$$P_{k}^{H} = \prod_{j \in J_{k}^{F}} \left(1 - p_{k,j}^{F} y_{k,j}^{F}\right) \sum_{j \in J_{k}^{H}} \left\{p_{k,j}^{H} y_{k,j}^{H} \left[\prod_{l \in J_{k}^{H}, l < j} \left(1 - p_{k,l}^{H} y_{k,l}^{H}\right)\right] \left[\prod_{m \in J_{k}^{H}, m > j} \left(1 - y_{k,m}^{H}\right)\right]\right\}, \quad k \in K$$

$$(38)$$

The probability of stage k to work at full capacity is calculated in equation (39), which is based on similar idea with that of equation (4) in section 5.1. However, in addition to the probability of total failure, probability of having half capacity also has to be deducted from 1.

$$P_k^F = 1 - \prod_{j \in J_k^F} \left(1 - p_{k,j}^F y_{k,j}^F\right) \prod_{j \in J_k^H} \left(1 - p_{k,j}^H y_{k,j}^F\right) - P_k^H, \quad k \in K$$
(39)

The probability of working with full capacity is the product of that of each stage.

$$A^F = \prod_{k \in K} P_k^F \tag{40}$$

The probability for the entire system to work under half throughput is represented as the probability for the system not to fail minus the probability of working with full capacity.

$$A^{H} = \prod_{k \in K} \left(P_{k}^{F} + P_{k}^{H} \right) - A^{F}$$
(41)

To account for partial capacity states, the availability of the system is redefined through the integration:

$$A = \frac{E}{\frac{u \in U}{CP^{f}T}} \left(\int_{0}^{T} CP(u, t) dt\right)}{CP^{f}T}$$

A conceptual graph is shown in Figure 7, where the availability equals the purple area over the rectangle area under the dashed line of full capacity. [0, T] is the time horizon that is being considered. CP^{f} is the full capacity of the system, and CP(t) is the system capacity at time t. However, only one scenario of the availability curve is shown in the figure, whereas in the defining equation, a probabilistic expectation is calculated, where u stands for each scenario and U stands for their set.



Thus, we can use equation (42) to estimate the system availability.

$$A = A^F + A^H/2 \tag{42}$$

In summary, the proposed non-convex MINLP model (TS) maximizes the net profit (9) subject to constraints (6)-(8), (13), (15), (18) - (20), (27) - (28) and (37)-(42).

6. Illustrative examples

In this section, several examples are presented and discussed in order to illustrate the applications of the models.

In section 6.1, we examine a system where all the stages have only two states, which was utilized to formulate a problem that maximizes the net profit, and a problem that maximizes reliability while minimizing cost. The single objective model (SO) was solved directly as a non-convex MINLP, and the multi-objective problem was solved by reformulating into its ϵ - constrained model (P1'), a non-convex MINLP, and then reformulated it as the convex MINLP (P1'L). In section 6.2, we formulate model (TS) to maximize the net profit for an ASU process where some of the stages may have three states, giving rise also to a non-convex MINLP. In section 6.3, availability evaluation is incorporated into the flowsheet superstructure optimization problem of methanol synthesis process and HDA (hydrodealkylation of toluene) process.

All models were implemented in GAMS 24.4.1 on an Intel(R) Core(TM) i7, 2.93GHz. Commercial solvers BARON 14.4.0 and DICOPT(based on CONOPT 3.16D and CPLEX 12.6.1.0) were used.

6.1. Binary state system

Figure 8 displays a simple serial system that has 4 stages with up to 3 units at each stage. Each rectangle represents a single processing unit. The parallel units in stage 1 and 2 are identical, respectively, while those in stages 3 and 4 are distinct. All of the stages are with binary states, giving rise to a total of 441 possible designs. Major parameters, including the availability, installation cost, and repair cost of each potential unit are given in Table 2.



Table 2: Parameters for example 1

	Ava	ilability		Insta	allation c	ost (K\$ pe	er year)	R	epair cost	(K\$ per	year)
	k=1	k=2	k=3		k=1	k=2	k=3		k=1	k=2	k=3
j=1	0.97	0.97	0.97	j=1	65	65	65	j=1	5	5	5
j=2	0.97	0.97	0.97	j=2	40	40	40	j=2	4	4	4
j=3	0.95	0.92	0.9	<i>j</i> =3	100	90	85	<i>j</i> =3	10	8	6
j=4	0.98	0.94	0.9	j=4	196	156	124	j=4	14	12	10

6.1.1. Net profit optimization

Model (SO) introduced in section 5.1.1 is applied to the above example and generates 29 equations, 26 variables with 13 discrete variables. It was solved by BARON in 0.405 s. The parameters for revenue, penalty and bonus to formulate the problem that maximizes the net profit are given in Table 3.

Table 3: Additional parameters for single objective model

rv (k\$/yr)	$pn \; (k\$/yr)$	bn ~(k\$/yr)	A_lo	$A_{-}up$
1000	800	800	0.988	0.996

The design decisions for maximizing the net profit are shown in Figure 9. A colored box indicates that the unit is selected to install, while a vacant space means that the unit is not selected.



The optimal design has an availability of 0.944, which is below the lower limit and incurs a \$52.3k/yr penalty. The system is expected to earn \$944.4k/yr of revenue with 0 bonus and \$52.3k/yr penalty, and to spend \$557k/yr on investment(including installation and repair), which results in the net profit of \$335.1k/yr.

6.1.2. ϵ -constrained model and its linearized formulation

Table 4 shows the Pareto results for the bi-criterion optimization problem. Two groups of MINLP's, the non-convex MINLP's (P1') and their linearized version, the convex MINLP's (P1'L)(described in section 5.1.2), were solved to identical results with the upper bound of the total cost varying by \$60K/yr from \$460K/yr to \$820K/yr respectively. Since the design decisions are discrete, the calculated values of C^{tot} might be less than the limit value.

Table 4: Pareto results

\overline{cost} (K\$/yr)	460	520	580	640	700	760	820
C^{tot} (K\$/yr)	436	480	571	622	692	692	819
A	0.849	0.900	0.947	0.951	0.975	0.975	0.993

Each point in Figure 10 corresponds to one of the six subproblems solved to maximum system availability under certain upper bound of total cost. The small chart next to each data point indicates the selected design decisions.



It is shown that as the upper bound of the cost increases, the maximum system availability increases as well. From Figure (10), we can also see the impact of the budget on the selection of the units for each stage. Generally speaking, the optimal designs for larger budgets have more units than those for smaller budgets. However, it is not merely a process of adding on units. As the upper bound of the total cost increases, some units are added, while some are discarded. Also note that the kinks in the Pareto curve are due to the changes in system configuration, and more fundamentally, the discrete nature of the problem. Table 5 compares the sizes and mean computational times of the models (P1') and (P1'L).

	No. Eq.	No. Var	No. Dis. Vars	Solver	Mean time
P1'	21	22	12	BARON	0.27s
P1'	21	22	12	SCIP	0.11s
P1'L	97	50	40	DICOPT	0.61s
P1'L	97	50	40	SBB	0.88s

Table 5: Computational statistics of (P1') and (P1'L)for example 1

For an expanded system (example 1') with 12 stages and 3 potential units for each stage giving rise to possible designs, the computational results are shown in Table 6.

Table 6: Computational statistics of (P1') and (P1'L) for example 1'

	No. Eq.	No. Var	No. Dis. Vars	Solver	Mean time
P1'	51	72	42	BARON	1.57s
P1'	51	72	42	SCIP	1.08s
P1'L	317	170	140	DICOPT	0.77s
P1'L	317	170	140	SBB	3.28s

Both (P1) and (P1'L) and their expanded system are solved using different solvers. As shown in the above tables, the size of (P1'L) is always larger than that of (P1'). From table 6, the mean solution time of (P1'L) on example 1 is longer than that of (P1'), regardless of solvers. However, the mean solution time of (P1'L) by DICOPT on the expanded example 1' is shorter than that of (P1') by either BARON or SCIP, which proves that the convexity of (P1'L) brings time efficiency for larger problems. The convexity of (P1'L) also guarantees that DICOPT can provide the global optimal solution. The solver SBB on the other hand is not able take advantage of convexity, for its computational time increases more rapidly with the number of binary variables as the NLP subproblems have to be solved at each node of the branch and bound tree. This example shows that the sacrificing of simplicity in exchange for convexity is not effective for all solvers.

6.2. Multi-state system (ASU)

As it can be seen, the motivating example of ASU units described in section 2 features multi-state behaviors (see Figure 11). Therefore, in this section, we will use it to illustrate the non-convex MINLP model (TS) (section 5.2).



Figure 11: The diagram of ASU reliability design alternatives

6.2.1. Optimal design

The model is first solved with the parameters shown in Table 7.

Table 7	Parameters	for	example	1
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	Availability			Installation cost $(M\$/yr)$				Repair cost $(k\$/yr)$					
	j = 1 $j = 2$	j = 3	j = 4		j = 1	j=2	j = 3	j = 4		j = 1	j=2	j = 3	j = 4
MAC	0.977 0.97	5 0.973		MAC	2	1.2	1.1		MAC	40	24	22	
PPF	0.995 0.99	3 0.991		PPF	1.6	1.5	1.4		PPF	32	30	28	
HEX	0.998 0.99	6 0.994	0.992	HEX	1.4	1.3	0.8	0.7	HEX	28	26	16	14
PUMP	0.968 0.96	6 0.965		PUMP	0.4	0.22	0.20		PUMP	8	4	4	
$rv = \$120M/yr, pn = \$130M/yr, bn = \$130M/yr, A_lo = 0.988, A_up = 0.996$													

Figure 12 shows the optimal configuration, which has a net profit of 105,898,000/yr and an availability of 0.970. The model has 29 equations, 38 variables with 16 discrete variables and was solved by BARON in 0.07 s



Figure 12: Optimum reliability design for multi-state ASU

6.2.2. Sensitivity Analysis

Unit availabilities

First, the values of unit availabilities are varied parametrically to evaluate their impact on the optimal design and the profitability of the system.



Figure 13: Net profit & system availability change with unit availabilities

In Figure 13 above, nominal value refers to the set of unit availability values used in section 6.2.1, Table 7. It is shown that as the availability values of single units are scaled down, the optimal net profit and system availability also decrease. The optimal designs are also changing in that more parallel units tend to be installed as unit availabilities decrease. A few representative structures are shown in the range considered for scaled availabilities.

When availabilities of single units in Table 7 increase by 0.02%, the optimal flowsheet does not differ from that with nominal values. However, since the units are more reliable, the optimal system availability and net profit do increase from \$105,898,000/yr to \$106,891,000/yr, and from 0.970 to 0.974, respectively.

When unit availabilities decrease by 1%, a standby heat exchanger is added on the flowsheet showed in Figure 14, with a system availability of 0.961 and net profit of \$102,438,000/yr.



Figure 14: Optimal flowsheet of ASU when availabilities decrease by 1% of nominal values

When unit availabilities decrease by 2% to 7%, the optimal flowsheet shown in Figure 15 has one more pump with half capacity than that shown in Figure 14. The optimal system availabilities for 2%, 5%, and 7% are 0.952, 0.918, and 0.894, with corresponding net profits of \$99,810,000/yr, \$91,384,000/yr, and \$85,335,000/yr.



Figure 15: Optimal flowsheet of ASU when availabilities decrease by 2%-7% of nominal values

When unit availabilities decrease by 8%, a standby heat exchanger is added on the flowsheet showed in Figure 14, with a system availability of 0.884 and net profit of \$82,240,000/yr.



Figure 16: Optimal flowsheet of ASU when availabilities decrease by 8% of nominal values

Contract-based penalty and bonus

Second, we analyze model sensitivity with respect to the contract-based penalty rate pn and bonus rate bn (first used in section 5.1.1). The trade-off between plant availability and investment is affected in the way that the higher these parameters are, the more important it becomes to increase plant availability, and thus, the more parallel units are to be installed.

When pn and bn are increased by 4 times, a pump with half capacity is added to the flowsheet, leading to a net profit of \$116,464,000/yr with an availability of 0.971.



Figure 17: Optimal flowsheet of ASU for pn =\$520M/yr, bn =\$520M/yr

When pn and bn are increased by 8 times, a standby heat exchanger is added on the flowsheet showed in Figure 17, leading to a net profit of \$116,696,000/yr with an availability of 0.972.



Figure 18: Optimal flowsheet of ASU for $pn = \frac{1040 \text{M/yr}}{\text{yr}}$, $bn = \frac{1040 \text{M/yr}}{\text{yr}}$

When pn and bn are increased by 16 times, one more air compressor of full capacity is added, leading to a net profit of \$116,733,000/yr with an availability of 0.973.



Figure 19: Optimal flowsheet of ASU for pn = 2080 M/yr, bn = 2080 M/yr

The above results show that higher penalty and bonus factors makes the flowsheets with higher availability more preferable.

6.3. Application to process synthesis problems

As stated in section 3, the previous models are based on a fixed serial diagram, and the availability of the system is simply the product of the availabilities of each stage (5) or the linear combination of the products (42). However, in this section, the reliability model is integrated in the superstructure optimization of process synthesis problems. In other words, the existence of some of the unit operations depends on the selection of a particular process flowsheet. A general disjunctive programming representation of a process synthesis problem (PS) is given as follows (Grossmann and Trespalacios, 2013):

$$\min \quad Z = \sum_{i} c_{i} + f(x)$$

s.t.
$$g(x) \leq 0$$

$$\begin{pmatrix} Y_{i} \\ h_{i}(x) \leq 0 \\ c_{i} = \gamma_{i} \end{pmatrix} \lor \begin{pmatrix} \neg Y_{i} \\ B^{i}x = 0 \\ c_{i} = 0 \end{pmatrix} \quad i \in D$$

$$\Omega(Y) = True$$

$$x \in R^{n}, c \geq 0, Y \in \{True, False\}^{m}$$

(PS)

In (PS), Y_i are boolean variables associated with the selection of certain equipment, x stand for continuous variables such as flowrates, temperatures and pressures, c_i represent fixed costs and f(x) are costs related to x. g(x) and $h_i(x)$ represent the equations and inequalities of the process.

To integrate reliability evaluations, each equipment in (PS) is considered as a stage, and parallel units are assigned for certain stages $i \in D^R$. Let the Boolean variables W and their corresponding binary variables w represent the existence of the parallel units. $\Omega(Y) = True$ becomes $\Omega(Y, W) = True$, where logical constraints relating the selection of stages and their parallel units are added; i.e., if the stage is not selected, its parallel units are not selected either. The availability evaluation model is represented by mixed-integer equations $c_i = \gamma_i(w)$ and $AV_i = P_i(w)$, where AV_i is the availability of stage *i*. Below is the general formulation of a process synthesis problem considering reliability (PSR).

$$\begin{array}{ll} \min & Z = \sum_{i} c_{i} + A \cdot f(x) \\ \text{s.t.} \\ g(x) \leq 0 \\ \begin{pmatrix} Y_{i} \\ h_{i}(x) \leq 0 \\ c_{i} = \gamma_{i} \end{pmatrix} \lor \begin{pmatrix} \neg Y_{i} \\ B^{i}x = 0 \\ c_{i} = 0 \end{pmatrix} \quad i \in D \backslash D^{R} \\ \begin{pmatrix} Y_{i} \\ h_{i}(x) \leq 0 \\ c_{i} = \gamma_{i}(w) \\ AV_{i} = P_{i}(w) \end{pmatrix} \lor \begin{pmatrix} \neg Y_{i} \\ B^{i}x = 0 \\ c_{i} = 0 \\ AV_{i} = 1 \end{pmatrix} \quad i \in D^{R} \\ \Omega(Y, W) = True \\ W \leftrightarrow w \\ A = \prod_{i \in D^{R}} AV_{i} \\ x \in R^{n}, c \geq 0, Y \in \{True, False\}^{m}, W \in \{True, False\}^{l} \end{array}$$

6.3.1. Methanol synthesis

In this section an example is presented to show the implementation of the availability modeling in the process design based on flowsheet superstructure optimization.



Figure 20: Superstructure of methanol synthesis process

The process synthesis problem of methanol synthesis process was formulated and solved as an MINLP by Türkay and Grossmann (1996) without reliability considerations based on the superstructure shown in Figure 20. Single choices have to be made regarding two feeds and two reactors. Feed 2 is more expensive but has less inert species than Feed 1. Reactor 2 is more expensive but has higher conversion than reactor 1. In addition, it has to be determined whether to use a single-stage compressors, or a two-stage compressor with intercooling for pressurization of the feed and the recycling stream respectively. The corresponding MINLP problem has 269 equations, 280 variables and 6 discrete variables and was solved with DICOPT (based on CONOPT 3.16D and CPLEX 12.6.1.0) in 0.343s for an optimal profit of \$3,684,468/yr. The corresponding optimal flowsheet (without guarantee of global optimality) is shown in Figure 21. According to the solution, Feed 1 is selected over Feed 2, and Reactor 1 is chosen rather than Reactor 2. In addition, one-stage compressor train is selected for the feed, and two-stage compressor train is selected for the recycling stream.



Figure 21: Optimal flowsheet of original methanol synthesis problem

In order to incorporate the availability evaluation, several candidate parallel units are assigned to each equipment with reliability considerations, such as compressors, heat exchangers and valves. Table 8 shows the equipment and parallel units, their capacities, and parameters of availabilities and costs. The equivalent reliability superstructure has 14 potential stages, with each of them having 3 to 4 potential parallel units, giving rise to a total of over 4 million design alternatives. The extended problem has 408 equations, 451 variables and 72 discrete variables and was solved by DICOPT in 0.452s to the optimal profit of \$3,404,302/yr. and an availability of 0.971.

Equipment		Installation costs (k\$/yr)	Repair costs (k\$/yr)	Availability	Capacity(%)
	1	0.132^{*} power (kw) + 13.5	4	0.977	100
COMP1 to COMP6	2	0.145^{*} power (kw) + 10.9	2.4	0.975	50
	3	0.145^{*} power (kw) + 10.9	2.4	0.973	50
	1	0.027^{*} heat (kw) + 39.2	2.8	0.998	100
UEC1 + UEC4	2	0.027^{*} heat (kw) + 39.2	2.8	0.996	100
IIECI to IIEC4	3	0.030^{*} heat (kw) + 21.2	1.6	0.994	50
	4	0.030^{*} heat (kw) + 21.2	1.6	0.992	50
	1	0.027^{*} heat (kw) + 39.2	2.8	0.998	100
HEII1 4. HEII9	2	0.027^{*} heat (kw) + 39.2	2.8	0.996	100
пепі ю пепэ	3	0.030^{*} heat (kw) + 21.2	1.6	0.994	50
	4	0.030^{*} heat (kw) + 21.2	1.6	0.992	50
	1	1	0.2	0.999	100
V	2	1	0.2	0.999	100
	3	1	0.2	0.999	100

Table 8: Availability evaluation module for methanol process

The solution to the optimization model with availability evaluation is shown in Figure 22. Compared to the original design shown in Figure 21, the compressor train of recycling stream is changed from two stage to single stage to save fixed cost and reduce failure. In terms of parallel unit selection, a parallel unit of half capacity is selected for the feed compressor. Also, all three parallel units for the pressure reducing valve are used because of low costs.



Figure 22: Optimal flowsheet of methanol synthesis process considering reliability

It is interesting to note that the profit drops significantly after reliability is incorporated in the model. With the same reliability data, the availability of the optimal configuration in Figure 21 without redundant units is 0.923, and its real profit considering failure is \$3,353,900/yr. This is 1.5% (\$50,402/yr) lower than that of the optimal design in Figure 22 with the incorporation of reliability (\$3,404,302/yr) which has an availability of 0.971.

6.3.2. Hydrodealkylation of toluene (HDA)

In this section another example is presented to show the incorporation of the availability modeling in the flowsheet superstructure optimization.



Figure 23: Super structure of HDA process

The process synthesis problem of hydrodealkylation of toluene (HDA) process was addressed by Kocis and Grossmann (1989) without reliability considerations based on the superstructure shown in Figure 23. An optimal flowsheet was obtained as shown in Figure 24. According to the solution, the hydrogen feed is purified before mixing with toluene feed. The isothermal reactor is selected rather than the adiabatic reactor. The separation train of the products includes stabilizing column, benzene column and flash 3. And the overhead of flash 1 rich with hydrogen is directly recycled without any further purification, while the hydrogen in the overhead of the stabilizing column is purged with methane. The problem has 719 equations, 726 variables and 16 discrete variables and was solved with DICOPT in 2.62s, yielding a profit of \$4,317,054/yr.



Figure 24: Optimal flowsheet for HDA original problem

In order to apply availability evaluation, several candidate parallel units are assigned to each equipment with reliability consideration, such as compressors, heat exchangers, pumps and valves. Table 9 shows the equipment, their capacities, and parameters of availabilities and costs. The equivalent reliability superstructure has 19 potential stages, with each of them having 2 to 4 potential parallel units, giving rise to a total of over 400 million design alternatives. The extended problem has 893 equations, 955 variables and 108 discrete variables and was solved with DICOPT (based on CONOPT 3.16D and CPLEX 12.6.1.0) in 10.14s, yielding a profit of \$3,972,785/yr.

Equipment		Installation costs (k\$/yr)	Repair costs (k\$/yr)	Availability	Capacity(%)
	1	0.132^* power(kw) + 13.5	4	0.977	100
COMP1 to COMP4	2	0.145^{*} power(kw) + 10.9	2.4	0.975	50
	3	0.145^{*} power(kw) + 10.9	2.4	0.973	50
	1	0.027*heat (w) + 39.2	2.8	0.998	100
UEC1 + 0 $UEC2$	2	0.027^{*} heat (kw) + 39.2	2.8	0.996	100
HECI to HECZ	3	$0.030^{\text{*}heat k(w)} + 21.2$	1.6	0.994	50
	4	0.030^{*} heat (kw) + 21.2	1.6	0.992	50
	1	0.027*heat (kw) + 39.2	2.8	0.998	100
HEH1 to HEHA	2	0.027*heat (kw) + 39.2	2.8	0.996	100
	3	0.030^{*} heat (kw) + 21.2	1.6	0.994	50
	4	0.030^{*} heat (kw) + 21.2	1.6	0.992	50
HEV	1	0.027^{*} heat (kw) + 39.2	2.8	0.988	100
IILA	2	0027*heat (kw) + 39.2	2.8	0.988	100
	1	1*flowrate(kg-mol/min)+1	0.2	0.968	100
PUMP1 to PUMP2	2	1.1*flowrate(kg-mol)+ 0.5	0.2	0.966	50
	3	1.1*flowrate(kg-mol)+ 0.5	0.2	0.964	50
V1 to V6	1	1	0.2	0.999	100
VI 00 V0	2	1	0.2	0.999	100

Table 9: Additive availability evaluation module

The optimal solution to the model with availability evaluation is shown in Figure 25, with a profit of \$3,972,785/yr and an availability of 0.942. The original problem with a profit of \$4,317,054/yr and not accounting for reliability, drops to a profit of \$3,817,535 considering failures (availability of 0.9045), which is 4% lower than the \$3,972,785/yr by the extended model. A half capacity standby is selected for COMP2. In addition, HEX, HEC1, V2, and V3 each has one full capacity standby unit. Comparing to the result shown in Figure 24, the purification step for hydrogen feed is skipped. Presumably, it is because the more complex routes do not provide enough additional profit that can balance the loss from higher possibility of failures and the costs from installing more parallel units. Therefore, the system tends to select simpler flowsheet structures to reduce failure and to retain sales revenue as much as possible.



Figure 25: Optimal flowsheet for HDA process considering reliability

7. Conclusion

This paper has presented MINLP models for selecting designs in serial systems to optimize their availability, where single units are given with fixed probabilities of being available. Two cases are investigated. For the first case, all the stages need only one unit to work properly. For the other case, some of the stages have two units sharing the workload. These stages provide half of the normal capacity when only one unit is left available, which gives the system an intermediate state besides merely up and down states.

Two non-convex MINLP models for maximizing system net profit were presented regarding the two cases. In addition, a non-convex ϵ -constraint MINLP model maximizing availability and minimizing cost separately was formulated for the first case, which can be reformulated as a convex MINLP. The application of these models was illustrated with several small examples. Furthermore, the availability evaluation was incorporated into flowsheet superstructure optimization problems for methanol synthesis process and hydrodealkylation process.

This work provides rigorous mixed-integer models for the general problems of optimal structural design of a reliable chemical process. The performance of the model on several examples has illustrated the potential of application on practical problems. On the other hand, the model has certain limitations, a most significant one of which is that it considers no maintenance. In regards to that, the authors will address in future work the approaches that are more simulation oriented in order to incorporate such issues.

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