MINLP models for optimizing availability in chemical plants with serial structure

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Abstract
Motivated by the reliability/availability concern in chemical plants, this paper proposes MINLP models that determine the optimal selection of parallel units to consider the trade-off between the availability of a serial producing system and the total costs. Both a basic scenario where the system transitions between only available and unavailable states, and an advanced scenario where the system has an intermediate state besides merely up and down are studied. Two non-convex MINLP models maximizing system net profit are introduced for the two situations respectively. In addition, a non-convex ϵ-constraint MINLP model maximizing availability subject to parametrically varying cost upper bound is posed for the first senario, which is then convexified. It is also proposed to add the availability evaluation part to process synthesis optimization problems over flowsheet superstructure. The model applications are illustrated with several examples which show that the computational requirements are small.

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 new plants, which 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 guarantee optimal solutions.

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 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 the measure/evaluation of system reliability, the detection of 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 multi-state 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 on 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. 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, reliability-based design optimization (RBDO) arises at the early stages for determining the topology and parameters of a system. Kuo and Prasad (2000) give an exhaustive 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 (Thomaidis and Pistikopoulos, 1994). Rudd (1962) discusses the estimation of system reliability with parallel redundancies. Henley and Gandhi (1975) suggest using minimal path method to evaluate failure propagation and the sensitivity of system reliability to unit reliability. Goel et al. (2003b) consider both design and planning of production and maintenance in an MILP model with variable reliability parameters and fixed system configuration. Terrazas-Moreno et al. (2010) use Markov process theory in an MILP model to optimize the selection of alternative plants and the design of intermediate storage for an integrated production site.

Currently, there are virtually no general mixed-integer programming models for optimal structural design of a reliable chemical process. This work considers a multi-objective optimization model to select parallel units in order to optimize availability and to minimize cost in serial systems.

2 Motivating example

To better focus on the parallel unit selection problem, we consider a rather simple flowsheet, an air separation unit (ASU) (Figure 1) as a motivating example. The production assets include air compressor, cooling, purification, distillation, etc.

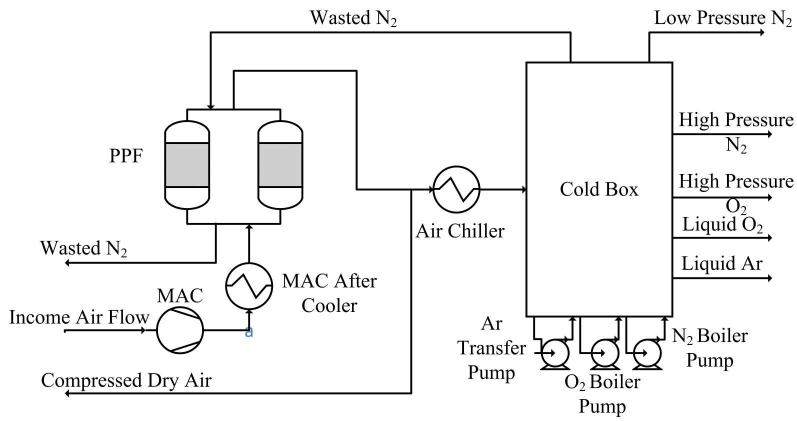


Figure 1: Typical flowsheet of air separation units

The failure of any one of the operations can result in the failure of the whole system. Thus, we formulate the process as a serial system of independent stages shown in the block diagram of Figure 2.

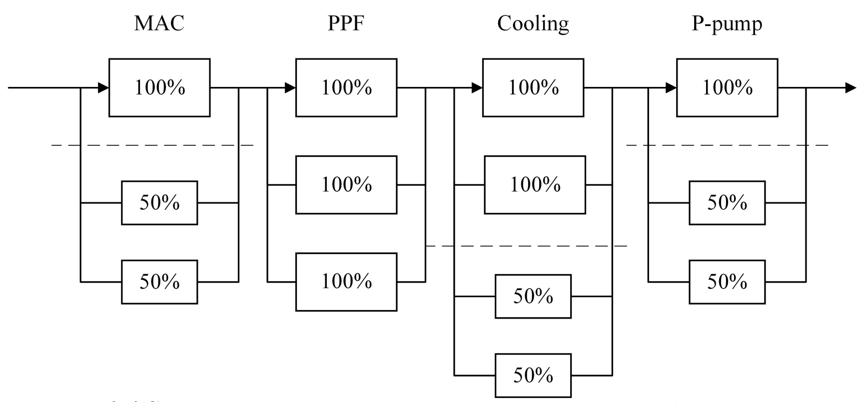


Figure 2: The diagram of ASU reliability design alternatives. Each block represents a parallel unit with certain rate of capacity shown in the block

3 Problem statement

In this section, we develop general models based on the serial system configurations (Figure 3) abstracted and generalized from the ASU case. The models make design decisions regarding whether to install each of the potential parallel units, in order to maximize the system availability (i.e. probability that the system performs without failures) and minimize the total cost of the entire system.

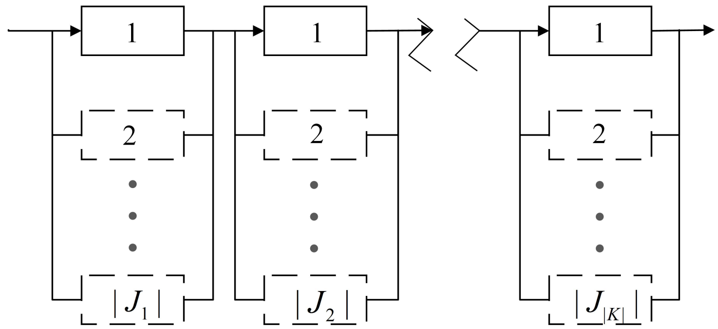


Figure 3: A serial system

Two kinds of situations are investigated. One of them is the basic scenario 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 certain availabilities (i.e. the probability of finding the unit 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, and cost rates. The stage k is considered fail where all its units are failed. The processing stages are divided into two kinds, stages where potential parallel units are completely identical ($k \in K_{iden}$), and stages where potential parallel units have the same capacities, but are distinct in terms of availability, cost, etc ($k \in K_{non}$).
In the other scenario being investigated, some of the stages may need one or two units to deliver full capacity. The model for the advanced scenario is built under similar frameworks, however, due to the existence of flexible stages (those who can have one or two necessary units), the stages are classified more particularly. A more fundamental difference is that the stages where two units are sharing the workload will 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.
Two non-convex MINLP models maximizing system net profit are presented in detail regarding the two situations respectively. In addition, considering maximizing availability and minimizing cost separately, another non-convex ϵ-constraint MINLP model that can be convexified for the basic scenario is posed. What's more, the possibility of combining this availability evaluation part with process synthesis problem over flowsheet superstructure is examined. Illustrative case studies are presented for all these models mentioned above.

4 Nomenclature

Indices

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

Set

K	Set of processing stage (e.g. absorption)
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

Parameter

n_k	Number of potential parallel units in stage k
p_k	Availability of single units in stage k with identical parallel units
$p_{k,j}$	Availability of single unit j in stage k with non-identical parallel units
c_inst_k	Investment for single units in stage k with identical parallel units
c_repa_k	Repair cost for single units in stage k with identical parallel units
$c\_inst_{k,,j}$	Investment for single unit j in stage k with non-identical parallel units
$c\_repa_{k,,j}$	Repair cost for single unit j in stage k with non-identical parallel units
$cost\_bar$	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

$y_{k,j}$	Binary variable that indicates whether unit j of stage k is selected
P_k	Availability of stage k
E_k	Expectancy of units being repaired of stage k
C_repa_k	Total repair cost for single units in stage k
C_k	Total cost for stage k
C^{tot}	Total cost of system
RV	Expected revenue
PN	Expected penalty
BN	Expected bonus
NP	Net profit
w_1, w_2, w_3	Binary variable that indicate which one of the ranges A falls in
A^1, A^2, A^3	Components of A for corresponding range
PN^1, PN^2, PN^3	Components of PN for corresponding components of A
BN^1, BN^2, BN^3	Components of BN for corresponding components of A

5 Model Formulation

5.1 Binary state

First we present the constraints of the multi-objective optimization problem (P1) that maximizes system availability while minimizing total cost. We then introduce its ϵ-constraint optimization problem (P1') in order to obtain the Pareto optimal solution.

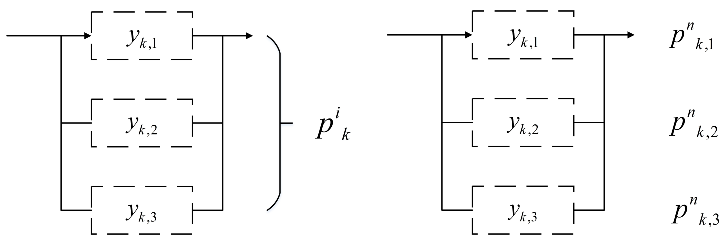
Constraint (1) requires that for each stage k at least one unit j should be installed.

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

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

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

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 scenarios for each stage to evaluate the availablity.



(a) Stage with identical units (b) Stage with distinct units

Figure 4: Sample diagrams for single stages

Consider the diagram in Figure 4(a) as an example, which has 4 scenarios in total: Unit 1 is active; Unit 2 is active while unit 1 has failed; Unit 3 is active while unit 1 and 2 have failed; All three units have failed. The first 3 scenarios correspond to the available state of the stage. Due to the symmetry breaking constraints (2), a unit j in stage k is selected means that all the potential units with higher priorities are in place. Therefore, whether a scenario is possible depends only on the existence of the unit that is active in it, and the probability for a possible scenario to take place depends on the availability of that particular unit as well as all the potential units with higher priorities. Thus, we have

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

which can be easily generalized to the form of equation (3).

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

The diagram in Figure 4(b) represents a stage $k \in K_{non}$ with non-identical redundancies, which is not restricted by symmetry breaking constraints. Hence, we cannot avoid nonlinearity by enumerating all the scenarios 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 scenarios. (Goel et al., 2003a)

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

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 cost.

$$C_k = (c\_inst_k + c\_repa_k) \sum_{j=1}^{n_k} y_{k,j}, \quad k \in K_{iden} \tag{6}$$

$$C_k = \sum_{j=1}^{n_k} y_{k,j} (c\_inst_{k,j} + c\_repa_k), \quad k \in K_{non} \tag{7}$$

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

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

A typical pattern of the way availability affecting net profit is applied 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 costs.

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

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

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

Since RV is positive in the maximized objective function (9), (10) can be relaxed as (11)

$$RV \le rvA \tag{11}$$

which can be converted to (12) based on the linearization presented in section 5.1.1 and (35)

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

Since $lnRV$ is concave separable, and $-\sum_{k\in K} lnP_k$ is convex, replacing (10) with (12) improves the quality of the feasible region and save the effort of spatial searching for global optimization.
Generally, in the contract between the plant and the customer, two reference bounds will be 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.

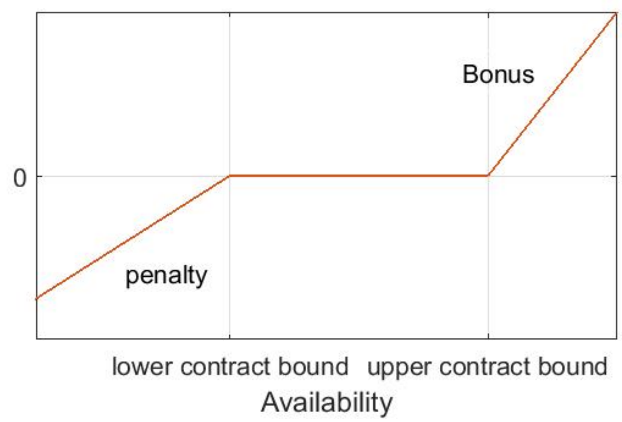


Figure 5: Definition of penalty and bonus functions

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

$$w_1 + w_2 + w_3 = 1 \tag{13}$$

$$\begin{pmatrix} w_1 = 1 \\ A \leq A\_lo \\ PN = (A\_lo - A)pn \\ BN = 0 \end{pmatrix} \vee \begin{pmatrix} w_2 = 1 \\ A\_lo \leq A \leq A\_up \\ PN = 0 \\ BN = 0 \end{pmatrix} \vee \begin{pmatrix} w_3 = 1 \\ A \geq A\_up \\ PN = 0 \\ BN = (A - A\_up)bn \end{pmatrix} \tag{14}$$

The convex-hull reformulation (Balas, 1985) yields,

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

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

$$BN = BN^1 + BN^2 + BN^3 \tag{17}$$

$$A^1 \leq w_1 A\_lo \tag{18}$$

$$w_2 A\_lo \leq A^2 \leq w_2 A\_up \tag{19}$$

$$A^3 \leq w_3 A\_up \tag{20}$$

$$PN^1 = (A\_low_1 - A^1)pn \tag{21}$$

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

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

$$BN = 0 \tag{24}$$

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

$$BN^3 = (A^3 - A\_upw_3)bn \tag{26}$$

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 MINLP (SO) maximizes the net profit (9) subject to (1)$-$(4), (6)$-$(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).

5.1.1 ϵ constrained model and convexified formulation

In stead 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 a remarkable property that it can be reformulated to a convex problem.

$$\max A \tag{29}$$

$$\min C^{tot} \tag{30}$$

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 (5) 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 Pareto-optimal curve.

$$C^{tot} \leq \cos t\_bar \tag{31}$$

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. Therefore, 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 be linearized. Since in (4), the multiplication was done over the set J_k, we first propose the following new sets and parameters to enumerate the subsets of J_k.
Set:

S Subset 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 $\mathbb{S}_1$ is $2^3 = 8$, $\mathbb{S}_1 = \{\varnothing, \{1\}, \{2\}, \{1, 2\}, \{3\}, \{1, 3\}, \{2, 3\}, \{1, 2, 3\}\}$.

The binary parameter $\alpha_{j,S}$ is defined to indicate whether unit j belongs to subset S: $\alpha_{j,S} = 1$ means that unit j belongs to subset S. Again, consider $J_1 = \{1, 2, 3\}$ as an example, then for $S = \{1, 2\}$, $\alpha_{1,S} = 1, \alpha_{2,S} = 1, \alpha_{3,S} = 0$. Table 1 gives a comprehensive example to show how $\alpha_{j,S}$ is defined for each alternative.m_S represents the order of S in $\mathbb{S}_k$

Table 1: An example of the correspondances between the indices of S and $\alpha_{j,S}$

$\alpha_{j,S}$			
		j	
m_S	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 $\mathbb{S}_k$, without any repetition or omission, we provide one way to generate the subsets automatically.

$$\alpha_{j,S} = \lfloor \frac{mod(m_S - 1, 2^j)}{2^{j-1}} \rfloor$$

Here $\alpha_{j,S}$ is the digit on the jth place of the binary form of $m_S - 1$
The following binary variables are then defined based on the above definition of S:

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

The following logic conditions hold for the $z_{k,S}$,

$$z_{k,S} \Leftrightarrow \Big(\bigwedge_{j \in S} y_{k,j} \Big), \quad k \in K_{non}, S \in \mathbb{S}_k, S \neq \varnothing$$

$$z_{k,S} = 1, \quad k \in K_{non}, S = \varnothing$$

which can be reformulated as the following linear inequalities,

$$z_{k,S} \leq y_{k,j}, \quad k \in K_{non}, j \in S, S \in \mathbb{S}_k, S \neq \varnothing \tag{32}$$

$$z_{k,S} \geq \sum_{j \in S} y_{k,j} - |S| + 1, \quad k \in K_{non}, S \in \mathbb{S}_k \tag{33}$$

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

$$\begin{aligned}P_k &= 1 - \prod_{j \in J_k} (1 - p_{k,j} y_{k,j}), \quad k \in K_{non} \\ &= 1 - \sum_{S \in \mathbb{S}_k} (\prod_{j \in S} (-p_{k,j} y_{k,j}))(\prod_{j \in J_k \backslash S} 1), \quad k \in K_{non} \\ &= 1 - \sum_{S \in \mathbb{S}_k} (\prod_{j \in S} (y_{k,j}))(\prod_{j \in S} -p_{k,j}), \quad k \in K_{non} \\ &= 1 - \sum_{S \in \mathbb{S}_k} z_{k,S} \prod_{j \in S} (-p_{k,j}), \quad k \in K_{non}\end{aligned} \tag{34}$$

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

$$\begin{aligned}P_1 = 1 - (z_{1,1} + z_{1,2}(-p_{1,1}) + z_{1,3}(-p_{1,2}) + z_{1,4}(-p_{1,1})(-p_{1,2}) + z_{1,5}(-p_{1,3}) \\ + z_{1,6}(-p_{1,1})(-p_{1,3}) + z_{1,7}(-p_{1,2})(-p_{1,3}) + z_{1,8}(-p_{1,1})(-p_{1,2})(-p_{1,3}))\end{aligned}$$

Thus, the expression of $P_k, k \in K$ are all linear in (P1L). On the other hand, let

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

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. Furthermore, for each single stage to be available, the least number of units that must be available is 1. However, in practice, most systems are subject to multi-state pattern. For simplicity, here in model (TS) we consider a representative situation, where for some stages at least 2 units are needed to operate at full capacity (if only one unit is available, the system has only half of the full capacity), for some stages at least 1 unit is needed, and some stages can choose either of the two patterns.

To account for the tri-state situation, we define new sets,

K_{ms}	Stages with three states
K_{bs}	Stages with only binary states
K_{mb}	Stages that can choose either pattern (flexible stages)
K^b_{iden}	Flexible stages whose units that serve in binary state pattern are identical
K^m_{iden}	Flexible stages whose units that serve in three state pattern are identical
K^b_{non}	Flexible stages whose units that serve in binary state are non-identical
K^m_{non}	Flexible stages whose units that serve in three state pattern are non-identical

New variables

x_b_k	Binary variable that indicates whether stage $k \in K_{mb}$ choose binary state pattern
x_m_k	Binary variable that indicates whether stage $k \in K_{mb}$ choose three state pattern
P_1_k	Probability of stage k working in full capacity
P_2_k	Probability of stage k working in half of full capacity
$P\_1^b_k$	Probability of stage $k \in K_{mb}$ working in full capacity when it chooses binary state pattern
$P\_2^b_k$	Probability of stage $k \in K_{mb}$ working in half of full capacity when it chooses binary state pattern
$P\_1^m_k$	Probability of stage $k \in K_{mb}$ working in full capacity when it chooses three state pattern
$P\_2^m_k$	Probability of stage $k \in K_{mb}$ working in half of full capacity when it chooses three state pattern
A_1	Probability of the whole system working in full capacity
A_2	Probability of the whole system working in half of full capacity

For stages with binary state, it is required that at least one unit is selected.

$$\sum_{j \in J_k} y_{k,j} \geq 1, \quad k \in K_{bs} \tag{37}$$

For stages with three states, it is required that at least two units be selected.

$$\sum_{j \in J_k} y_{k,j} \geq 2, \quad k \in K_{ms} \tag{38}$$

For stages that can choose,

$$x\_b_k + x\_m_k = 1, \quad k \in K_{bm} \tag{39}$$

$$x\_b_k \leq \sum_{j \in J^b_k} y_{k,j} \leq |J^b_k| x\_b_k, \quad k \in K_{bm} \tag{40}$$

$$2x\_m_k \leq \sum_{j \in J^m_k} y_{k,j} \leq |J^m_k| x\_m_k, \quad k \in K_{bm} \tag{41}$$

The symmetry breaking constraint for stages with identical parallel units (constraint (2)) still applies. For stages with only binary states, the availability of the stage is calculated as in previous models

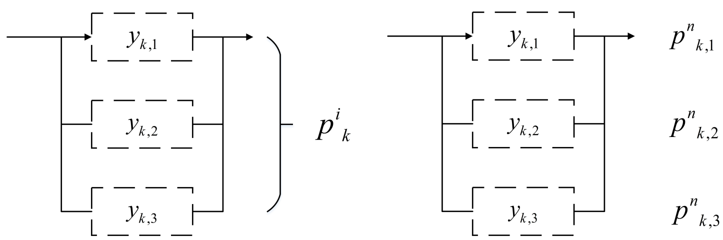
$$P\_1_k = p_k \sum_{j \in J_k} y_{k,j}(1-p_k)^{j-1}, \quad k \in K_{iden} \cap K_{bs} \tag{42}$$

$$P\_1_k = 1 - \prod_{j \in J_k} (1 - p_{k,j} y_{k,j}), \quad k \in K_{non} \cap K_{bs} \tag{43}$$

$$P\_1^b_k = p_k \sum_{j \in J^b_k} y_{k,j}(1-p_k)^{j-1}, \quad k \in K^b_{iden} \cap K_{mb} \tag{44}$$

$$P\_1^b_k = 1 - \prod_{j \in J^b_k} (1 - p_{k,j} y_{k,j}), \quad k \in K^b_{non} \cap K_{mb} \tag{45}$$

For stages with an intermediate state, there are two units working at the same time in each scenario. The scenarios are counted first in terms of the one with lower priority, then in terms of the one with higher priority.



(a) Stage with identical units (b) Stage with distinct units

Figure 6: Sample diagrams for single stages

Consider the diagram in Figure 6(a) as an example. Since the units are identical, the first two units must be installed. Thus, a case that must be taken into consideration is that the first two units are available and active at the same time. Then, if the third unit is selected, which is indicated by the binary variable $y_{1,3}$, there will be two other available cases, in both of which unit 3 is active, and either unit 1 or 2 is failed.

$$P\_1_1 = p_1^2 + 2p_1^2(1-p_1)y_{1,3}$$

This equation can then be generalized to the form of Equation (46) and (47)

$$P\_1_k = p_k^2 (1 + \sum_{j \in J_k, j \geq 3} y_{k,j}(1-p_k)^{j-2}(j-1)), \quad k \in K_{iden} \cap K_{ms} \tag{46}$$

$$P\_1^m_k = p_k^2 (1 + \sum_{j \in J^m_k, j \geq 3} y_{k,j}(1-p_k)^{j-2}(j-1)), \quad k \in K^m_{iden} \cap K_{mb} \tag{47}$$

For the stage shown in Figure 6(b), where the potential units are distinct, the available cases are the same as those listed for Figure 6. However, here the potential units are not selected in sequence, thus, more binary variables are multiplied to indicate the existence of the units.

$$P\_1_1 = p_{1,2}y_{1,2}p_{1,1}y_{1,1} + p_{1,3}y_{1,3}p_{1,1}y_{1,1}(1-p_{1,2}y_{1,2}) + p_{1,3}y_{1,3}p_{1,2}y_{1,2}(1-p_{1,1}y_{1,1})$$

Equation (48) and (49) is the generalized form of the above equation.

$$P\_1_k = \sum_{j\in J_k, j\geq 2} p_{k,j}y_{k,j}\sum_{i=1}^{j-1} p_{k,i}y_{k,i}\prod_{l=1,l\neq i}^{j-1}(1-p_{k,l}y_{k,l}), \quad k\in K_{non}\cap K_{ms} \tag{48}$$

$$P\_1_k^m = \sum_{j\in J_k^m, j\geq 2} p_{k,j}y_{k,j}\sum_{i=1}^{j-1} p_{k,i}y_{k,i}\prod_{l=1,l\neq i}^{j-1}(1-p_{k,l}y_{k,l}), \quad k\in K_{non}^m\cap K_{mb} \tag{49}$$

The scenarios providing half throughput for stages with multiple states will only happen when there is only one unit left available. A problem here is how to identify the unit with lowest priority among those that are selected. For identical-standby stages, the unit j if selected, is defined as the one installed with lowest priority as long as the unit $j+1$ is not selected, while for stages with distinct components, unit j is with the lowest priority among all existing units only if all the potential units $j+1, j+2, \ldots, n_k$ are not installed.

$$P\_2_k = \sum_{j\in J_k, j\geq 2} y_{k,j}p_k(1-p_k)^{j-1}(1-y_{k,j+1}), \quad k\in K_{iden}\cap K_{ms} \tag{50}$$

$$P\_2_k^m = \sum_{j\in J_k^m, j\geq 2} y_{k,j}p_k(1-p_k)^{j-1}(1-y_{k,j+1}), \quad k\in K_{iden}^m\cap K_{mb} \tag{51}$$

$$P\_2_k = \sum_{j\in J_k, j\geq 2} y_{k,j}p_{k,j}(\prod_{l=1}^{j-1}(1-p_{k,l}y_{k,l}))(\prod_{l=j+1}^{n_k}(1-y_{k,l})), \quad k\in K_{non}\cap K_{ms} \tag{52}$$

$$P\_2_k^m = \sum_{j\in J_k^m, j\geq 2} y_{k,j}p_{k,j}(\prod_{l=1}^{j-1}(1-p_{k,l}y_{k,l}))(\prod_{l=j+1}^{n_k}(1-y_{k,l})), \quad k\in K_{non}^m\cap K_{mb} \tag{53}$$

$$P\_2_k = 0, \quad k\in K_{bs} \tag{54}$$

$$P\_2_k^b = 0, \quad k\in K_{mb} \tag{55}$$

The availabilities of flexible stages are calculated as follows

$$P\_1_k = P\_1_k^b x\_b_k + P\_1_k^m x\_m_k, \quad k\in K_{mb} \tag{56}$$

$$P\_2_k = P\_2_k^b x\_b_k + P\_2_k^m x\_m_k, \quad k\in K_{mb} \tag{57}$$

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

$$A\_1 = \prod_{k\in K} P\_1_k \tag{58}$$

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

$$A\_2 = \prod_{k\in K}(P\_1_k + P\_2_k) - A\_1 \tag{59}$$

The availability is defined through the integration:

$$A = \frac{\underset{u \in U}{E}(\int_0^T CP(u,t)dt)}{CP^f T}$$

where $[0, T]$ is the production time that is considered. CP^f is the full capacity of the system, and $CP(t)$ is the system capacity at time t. Thus, we can use equation (60) to estimate the system availability.

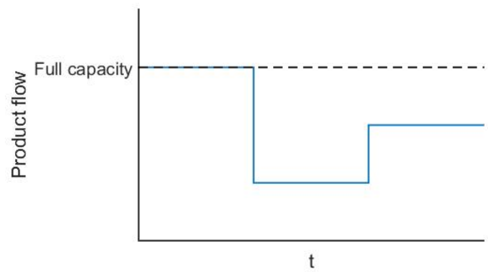


Figure 7: Sketch of an availability curve

$$A = A\_1 + A\_2/2 \tag{60}$$

In summary, the proposed non-convex MINLP model (TS) maximizes the net profit (9) subject to (6)−(8), (13), (15), (18) − (20), (37)−(60) and (27) − (28).

6 Illustrative examples

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

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 through reformulating into its ϵ- constrained model (P1'), a non-convex MINLP, and then reformulate 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 6.3.2, an availability evaluation part is added to an HDA (hydrodealkylation of toluene) process synthesis problem.

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. Major parameters including the availability, installation cost and repair cost of each potential unit are given in Table 2.

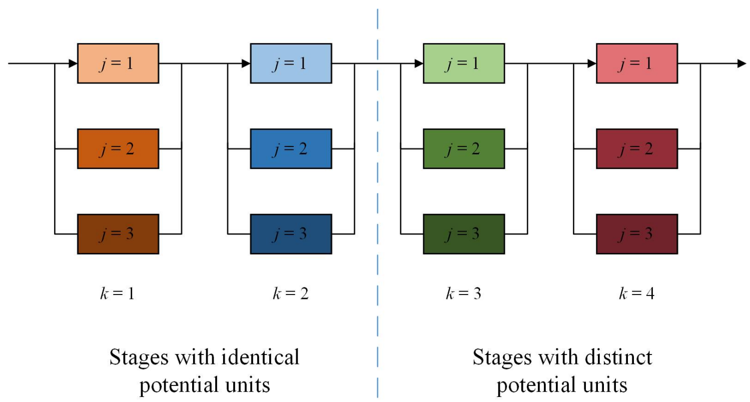


Figure 8: Example 1

Table 2: Parameters for example 1

	Availability				Installation cost				Repair cost		
	1	2	3		1	2	3		1	2	3
1		0.97		1		50		1		20	
2		0.97		2		40		2		4	
3	0.95	0.92	0.9	3	80	70	65	3	30	28	26
4	0.98	0.94	0.9	4	150	120	90	4	60	48	44

6.1.1 Net profit optimization

The rates for revenue, penalty and bonus are needed to formulate the problem that maximizes the net profit, which are displayed in Table 3. The model has 29 equations, 26 variables with 13 discrete variables. It was solved by BARON in 0.405 s.

Table 3: Additional parameters for single objective model

rv	pn	bn	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.

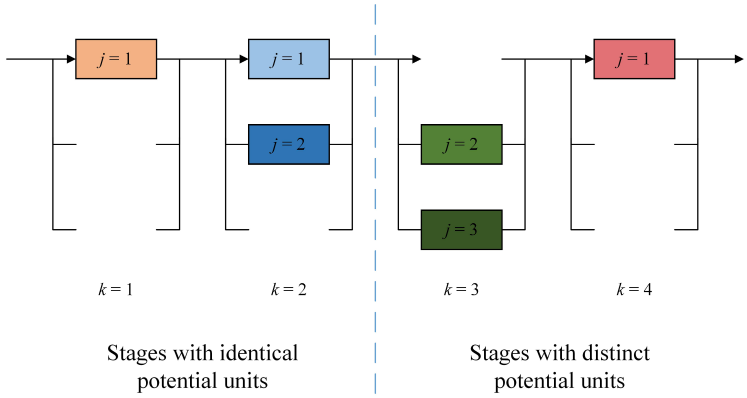


Figure 9: Optimization result of example 1

In the optimized case, the system is expected to earn 988.2 of revenue with 0 bonus and 0 penalty, and 833 on investment(including installation and repair). The net profit is 155.2.

6.1.2 ϵ-constrained model and its linearized formulation

Next in Table 4, we present the Pareto results for the multi-objective problem. Two groups of MINLP's were solved with the upper bound of the total cost varying by 60 from 460 to 820 respectively. The results of the non-convex MINLP's (P1') and their linearized version, the convex MINLP's (P1'L) are identical. Since the design decisions are discrete, the calculated values of C^{tot} might be less than the limit value.

Table 4: Pareto results

cost_bar	460	520	580	640	700	760	820
C^{tot}	436	480	571	622	692	692	819
A	0.849	0.900	0.947	0.951	0.975	0.975	0.993

In Figure 10, the small charts next to each data point indicates the selected design decisions.

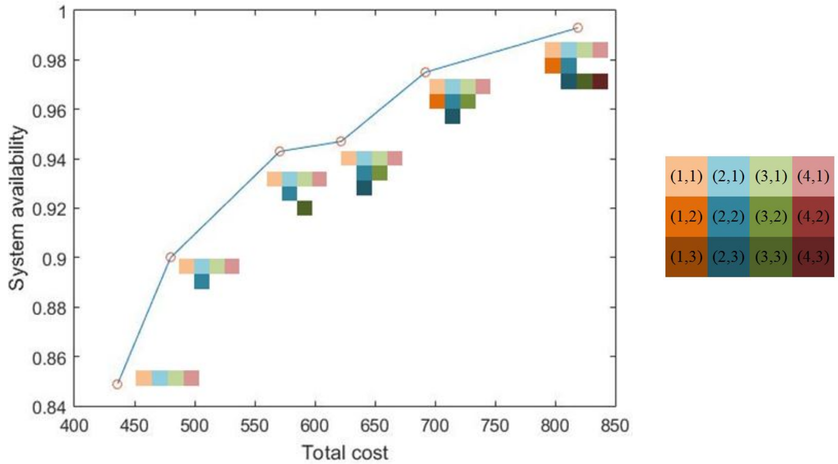


Figure 10: Pareto curve

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 computational results of single models (P1') and (P1'L).

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

	No. Eq.	No. Var	No. Dis. Vars	Solver	Mean time
P1'	21	22	12	BARON	0.038s
P1'	21	22	12	SCIP	0.016s
P1'L	97	50	40	DICOPT	0.087s
P1'L	97	50	40	SBB	0.125s

If we duplicate each stage three times and consider the expanded system (example 1') with 12 stages in total, the computational results are as shown in Table 6.

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

	No. Eq.	No. Var	No. Dis. Vars	Solver	Mean time
P1'	21	22	12	BARON	0.140s
P1'	21	22	12	SCIP	0.129s
P1'L	97	50	40	DICOPT	0.107s
P1'L	97	50	40	SBB	5.738s

Clearly, the scale of problem (P1'L) is larger than that of (P1'), and the average solving time of (P1'L) on example 1 is longer than that of (P1'). However, the average solving time of

(P1'L) on example 1' is shorter than that of (P1'), which proves that the convexity of (P1'L) brings it time efficiency that becomes more and more considerable for larger problems.

6.2 Multi-state system (ASU)

In this section we inspect again the ASU case that served as a motivating example in section 2. Non-convex MINLP(TS) is implemented for its design optimization.

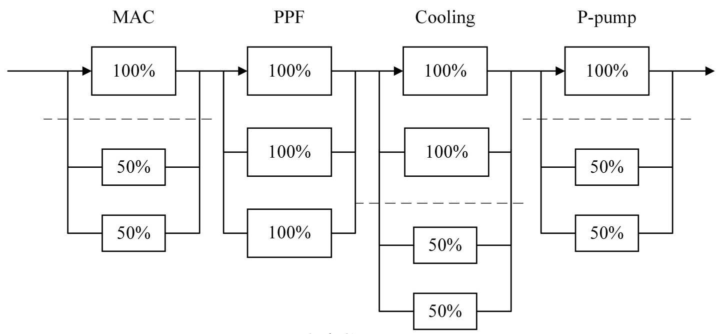


Figure 11: The diagram of ASU reliability design alternatives

Table 7 shows the parameters. There are no non-identical parallel units considered.

Table 7: Parameters of ASU example

	Availability			Installation cost			Repair cost	
	2-state part	3-state part		2-state part	3-state part		2-state part	3-state part
1	0.998	0.996	1	120	60	1	20	18
2	0.98		2	50		2	8	
3	0.992	0.990	3	100	50	3	30	20
4	0.996	0.993	4	20	10	4	5	3

$rv = 1000$, $pn = 800$, $bn = 800$, $A\_lo = 0.988$, $A\_up = 0.996$

Figure 12 shows the optimization result.

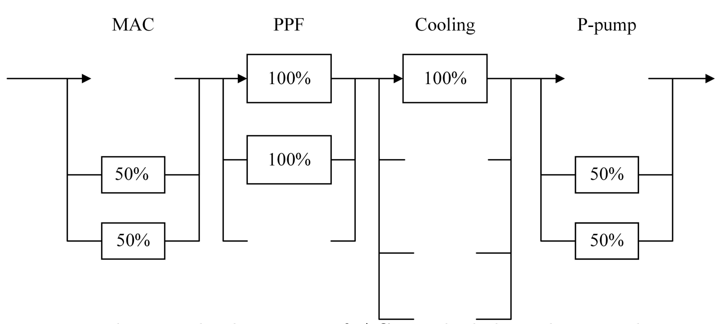


Figure 12: The result diagram of ASU reliability design alternatives

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 (60). However, in this section, the reliability model will be rendered a complementary part to normal process synthesis problems. In other words, the existence of some of the unit operations are not deterministic. To elaborate, a general disjunctive programming representation of a process synthesis problem (PS) is shown below:

$$
\begin{aligned}
&\min \quad Z = \sum_i c_i + f(x) \\
&\text{s.t.} \\
&g(x) \leq 0 \\
&\begin{pmatrix} Y_i \\ h_i(x) \leq 0 \\ c_i = \gamma_i \end{pmatrix} \vee \begin{pmatrix} \neg Y_i \\ B^i x = 0 \\ c_i = 0 \end{pmatrix} \quad i \in D \\
&\Omega(Y) = True \\
&x \in R^n, c \geq 0, Y \in \{True, False\}^m
\end{aligned}
\tag{PS}
$$

Here Y_i are boolean variables associated with the existence of units. x stand for continuous variables such as flowrates, temperatures, pressures, etc. c_i represent fixed costs and $f(x)$ are costs related to x.

To apply reliability evaluations, each unit in (PS) is taken as a stage, and parallel units are assigned for certain stages $i \in D^R$. Let boolean variables W and their corresponding binary variables w represent the existence of the parallel units. x^R are continuous variables related to stage and system availabilities including γ_i and P_i. AV_i is the availability of stage i. Then $AV_i = P_i$ when stage i exists, and 1 when it does not. Below is the general representation of a process synthesis problem considering reliability (PSR).

$$
\begin{aligned}
&\min \quad Z = \sum_i c_i + Af(x) \\
&\text{s.t.} \\
&g(x) \leq 0 \\
&g^R(x^R, w) \leq 0 \\
&\begin{pmatrix} Y_i \\ h_i(x) \leq 0 \\ c_i = \gamma_i \end{pmatrix} \vee \begin{pmatrix} \neg Y_i \\ B^i x = 0 \\ c_i = 0 \end{pmatrix} \quad i \in D/D^R
\end{aligned}
\tag{PSR}
$$

$$
\begin{pmatrix} Y_i \\ h_i(x) \le 0 \\ c_i = \gamma_i \\ AV_i = P_i \end{pmatrix} \vee \begin{pmatrix} \neg Y_i \\ B^i x = 0 \\ c_i = 0 \\ AV_i = 1 \end{pmatrix} \quad i \in D^R
$$

$$
\Omega(Y) = True
$$

$$
\Phi(W) = True
$$

$$
A = \prod_{i \in D^R} AV_i
$$

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

$$
x^R \in R^a, W \in \{True, False\}^b
$$

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.

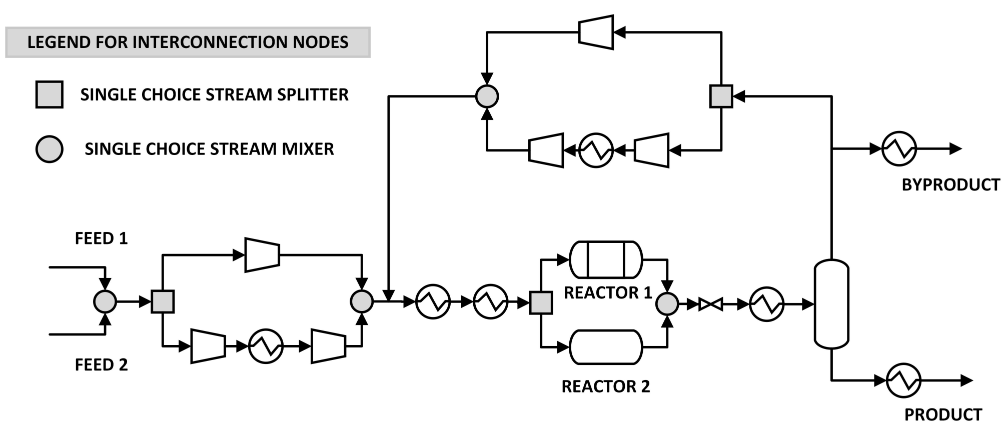


Figure 13: Supper structure of methanol synthesis process

The process synthesis problem of methanol synthesis process was solved as an MINLP by Türkay and Grossmann (1996) without reliability considerations based on the superstructure shown in Figure 13. 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 the two pressurization process respectively. A locally optimal flowsheet was obtained as shown in Figure 14. The problem has 269 equations, 280 variables and 6 discrete variables and was solved by DICOPT in 0.56s to the optimal profit of $4662.1K.

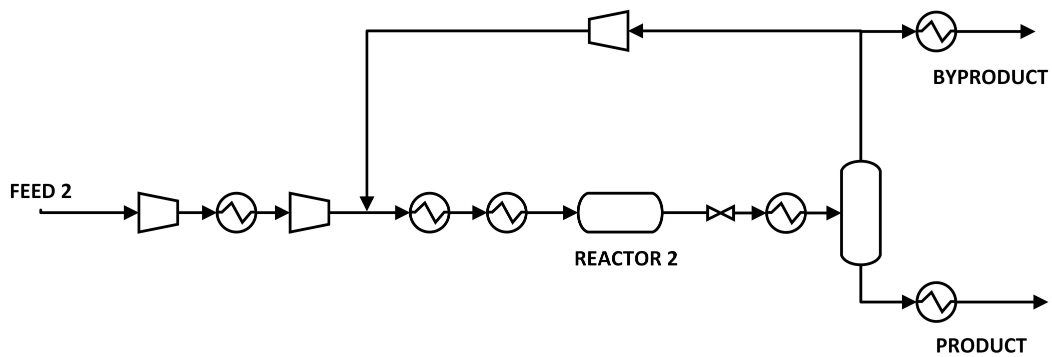


Figure 14: Result of original methanol synthesis problem

In order to apply availability evaluation, 3 identical potential parallel units are assigned to each selected unit operations such as compressors, heat exchangers and valves. Table 8 shows the selected unit operations, their incoming streams and parameters of availabilities and costs. The extended problem has 390 equations, 379 variables and 56 discrete variables and was solved by DICOPT in 0.94s to the optimal profit of $3964.4 K.

Table 8: Additive availability evaluation module

Unit operations		Stages	Incoming streams	Installation costs ($10^3 yr^{-1}$)	Repair costs ($10^3 yr^{-1}$)	Availability
compressor	1	1	4	0.068*power (kw) + 5.6	Installation cost/6	0.987
	2	2	5			0.987
	3	3	5			0.987
	4	4	27			0.987
	5	5	28			0.987
	6	6	28			0.987
cooler	1	7	5	0.0167*heat (kw) + 0.47	Installation cost/6	0.992
	2	8	11			0.992
	3	9	12			0.992
	4	10	19			0.992
heater	1	11	22	0.0167*heat (kw) + 0.47	Installation cost/6	0.992
	2	12	24			0.992
	3	13	30			0.992
valve	1	14	18	0.001	0.000	0.983

The solution to the model with availability evaluation is as shown in Figure 15. A flowsheet is selected and certain numbers of parallel units are kept for the stages being considered and remain in the resulting flowsheet.

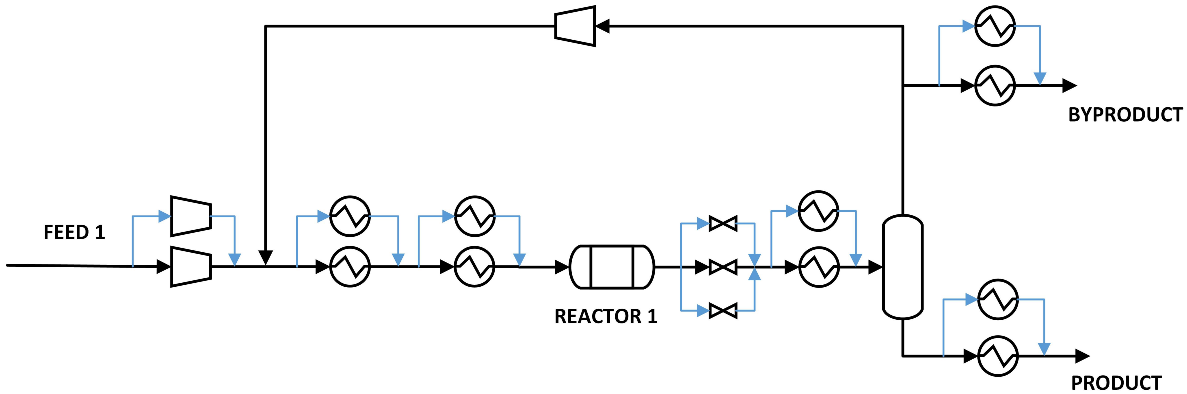


Figure 15: Result of methanol synthesis process considering reliability

The two-stage compressor before the recycle point is replaced by a single stage compressor to lower the probability of failure. The switch from expensive feed and reactor to cheaper ones can only be explained has a side product of the changes resulted by the extended part. It may have caught attention that the profit has dropped sharply after reliability module is introduced. However, with the same reliability data, the availability of the optimal configuration without redundant units is only 0.8591, and its real profit considering failure is $3949.8 K, which is lower than that of the problem with reliability part.

6.3.2 Hydrodealkylation of toluene (HDA)

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

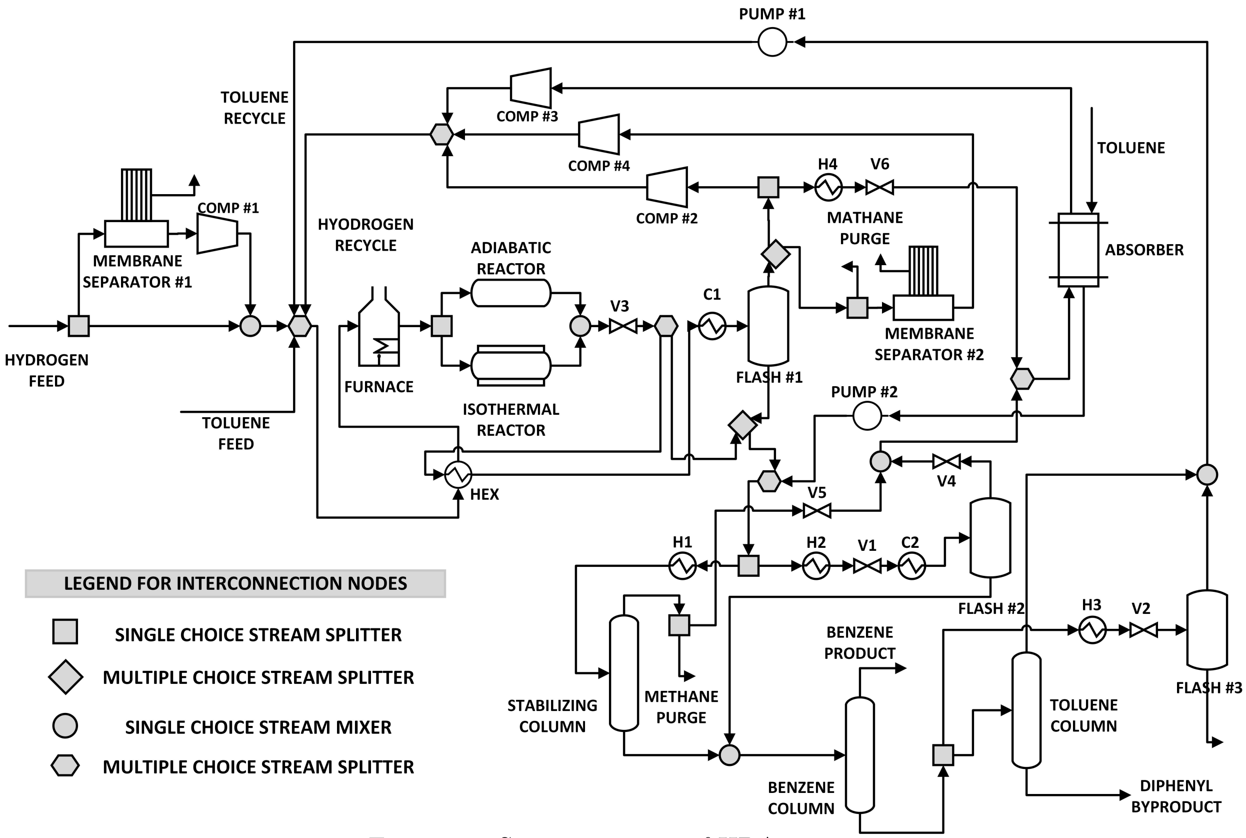


Figure 16: Super structure of HDA process

The process synthesis problem of hydrodealkylation of toluene (HDA) process was solved by Kocis and Grossmann (1989) without reliability considerations based on the superstructure shown in Figure 16. A locally optimal flowsheet was obtained as shown in Figure 17. According to the solution, it is decided to purify the hydrogen feed before mixing with toluene feed. The isothermal reactor is preferred 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 hyodrogen 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, 723 variables and 13 discrete variables and was solved by DICOPT in 2.05s.

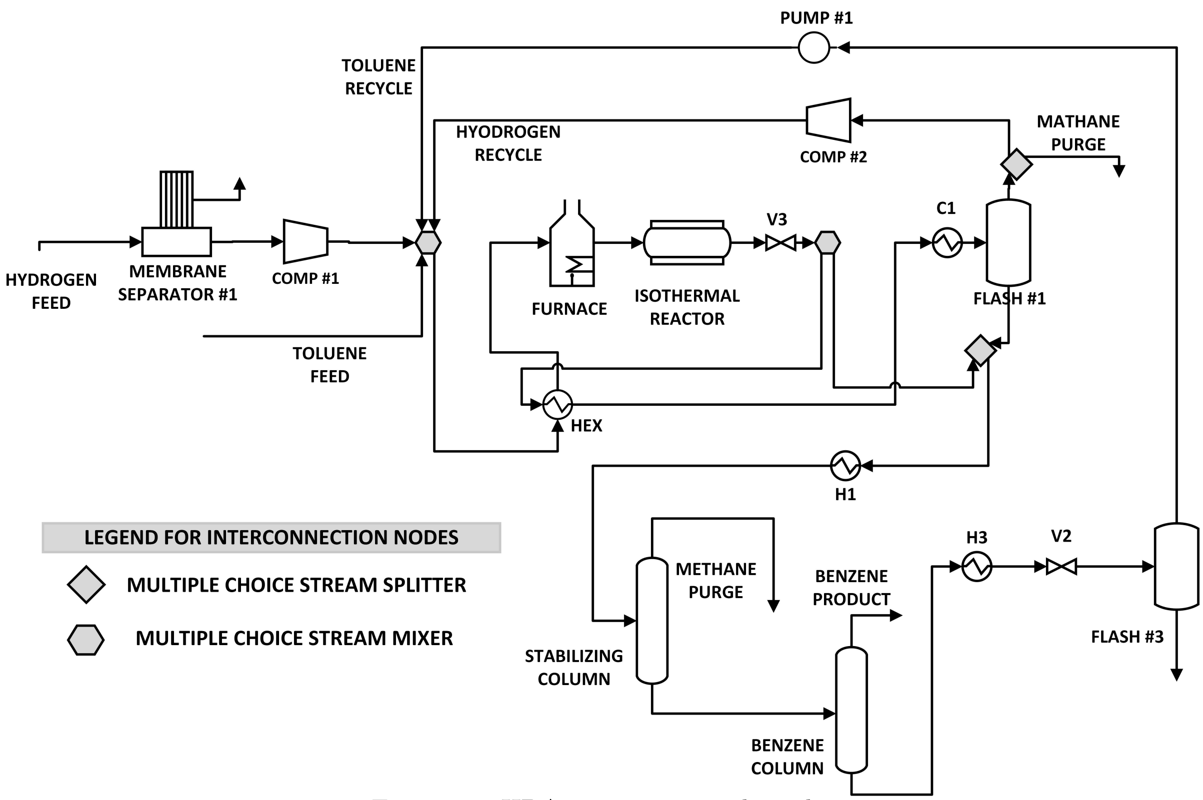


Figure 17: HDA process original result

In order to apply availability evaluation, 3 identical potential parallel units are assigned to each selected unit operations such as compressors, heat exchangers, pumps and valves. Table 9 shows the selected unit operations, their incoming streams and parameters of availabilities and costs. The extended problem has 892 equations, 858 variables and 89 discrete variables and was solved by DICOPT in 2.95s.

Table 9: Additive availability evaluation module

Unit operations		Stages	Incoming streams	Installation costs ($10^3 yr^{-1}$)	Repair costs ($10^3 yr^{-1}$)	Availability
compressor	1	1	5			0.987
	2	2	59	0.815*power (kw) + 7.155	Installation cost/6	0.987
	3	3	64			0.987
	4	4	56			0.987
cooler	1	5	71	1	0.167	0.97
	2	6	45	1	0.167	0.97
heater	1	7	24	1	0.167	0.97
	2	8	23	1	0.167	0.97
	3	9	37	1	0.167	0.97
	4	10	61	1	0.167	0.97
heat exchanger	1	11	8	1.5	0.25	0.989
pump	1	12	42	0.2	0.033	0.975
	2	13	68	0.2	0.033	0.975
valve	1	14	44	0.05	0.008	0.96
	2	15	38	0.05	0.008	0.96
	3	16	14	0.05	0.008	0.96
	4	17	47	0.05	0.008	0.96
	5	18	29	0.05	0.008	0.96
	6	19	73	0.05	0.008	0.96

The solution to the model with availability evaluation is as shown in Figure 18. A flowsheet is selected and certain numbers of parallel units are kept for the stages being considered and remain in the resulting flowsheet.

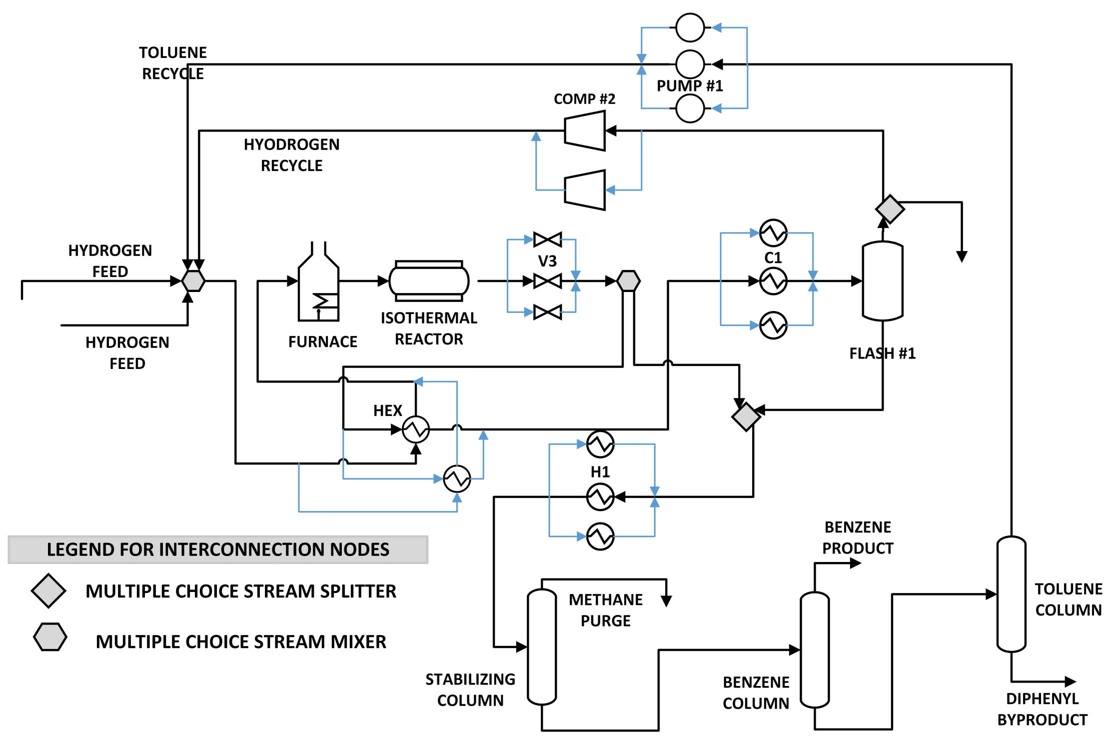


Figure 18: Result of HDA process considering reliability

Comparing to result shown in Figure 17, now the purification step for hydrogen feed is skipped, and flash 3 is replaced by toluene column. Curious enough, it appears that all the routes selected here tend to have fewer stages bearing availability considerations than their competitors. Arguably, it is because the more complex routes won't provide excess profits enough to balance the loss from higher possibility of failures and the costs from installing more parallel units. Thus, the system tends to adopt simpler flowsheet to reduce failure and to retain sales revenue as much as possible. The original problem is solved to a profit of \$4619.2 K and will drop to \$3842.1 K considering failures, comparing to \$4580.1 K by the model with reliability part.

7 Conclusion

Assuming that single units are given with fixed probabilities of being available, MINLP models have been presented for selecting designs in serial systems to optimize their availability. Two kinds of situations are investigated. For the first situation, all the stages need only one unit to work properly. For the other situation being investigated, some of the stages have two units sharing the workload. These stages will 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. Two non-convex MINLP models maximizing system net profit are discussed regarding the two situations respectively. In addition, another non-convex ϵ-constraint MINLP model maximizing availability and minimizing cost separately is posed for the first senario. It can be reformulated to a convex MINLP. What's more, the availability evaluation part is added to process synthesis optimization problems over flowsheet superstructure. As for future work, storage has not yet considered, which plays important part in guaranteeing the availability of a chemical plant. Furthermore, we will introduce Markov chain theory to account for the time-dependence of the system, in order to design storage capacities as well as taking care of various options at the process level.

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