MINLP models for optimal design of reliable chemical plants

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Abstract

This paper proposes a multi-objective optimization model (P1) that determines the optimal selection of parallel units considering the trade-off between the availability of a serial producing system and total investment costs. Model (P1) is solved through the ϵ- constrained MINLP model (P1') that maximizes system availability subject to a series of upper bounds of the total cost, which yields a set of Pareto-optimal solutions. Convexification to (P1'L) through exact linearization of the constraints and substitution of the objective function is also presented. Application of the model is illustrated with an example which shows the capabilities of the model and that the computational requirements are small.

Keywords

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

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 chemi-

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cal 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.

Motivating example

To motivate the need for systematic optimization models for availability, we consider an air separation unit (ASU) as shown in Figure 1. The production assets include air compressor, cooling, purification, distillation, etc.

We consider the case when there is no storage. In that case the failure of any one of the operations can result in the failure of the whole system. Despite the complex configuration of the process flowsheet, one can formulate the process as a serial system of independent stages as shown in Figure 2 (Goel et al., 2003a), where the design alternatives are also shown in the form of standby or parallel units with percentages of capacities marked on the blocks. The objective is to maximize the availability of the plant while constraining the total cost.

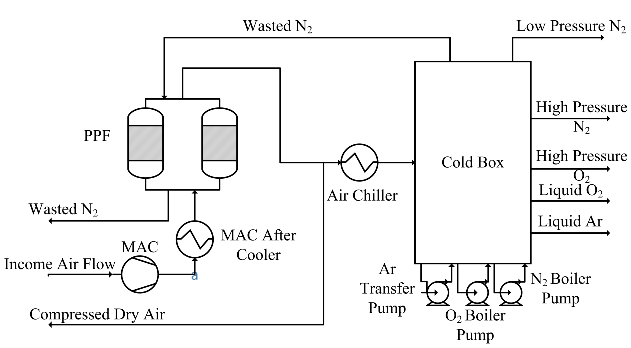


Figure 1. Typical flowsheet of air separation units

Problem statement

In this section, we develop a new general model based on abstract configurations as shown in Figure 3, which can be applied for instance to the ASU case.

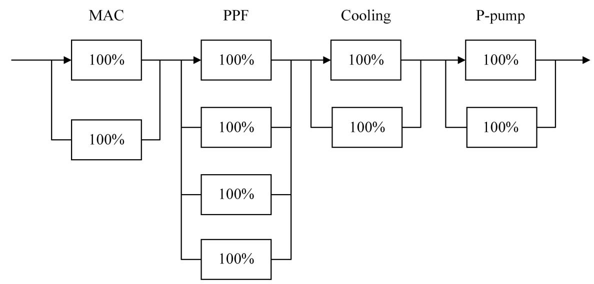


Figure 2. The diagram of ASU reliability design alternatives

A set of potential units $j \in J_k$ for each stage k are given with fixed availabilities, cost rates, and operating priorities(indicated by j), which means that a unit can only be active when all installed units that have higher priorities fail (see Figure 3). When the number of available units is less than one, the stage is considered to have failed. The system has two kinds of processing stages, stages where potential parallel units are identical ($k \in K_{iden}$), and stages where potential parallel units have the same capacities, but are distinct in terms of availability, cost, etc ($k \in K_{non}$)(see Figure 4).

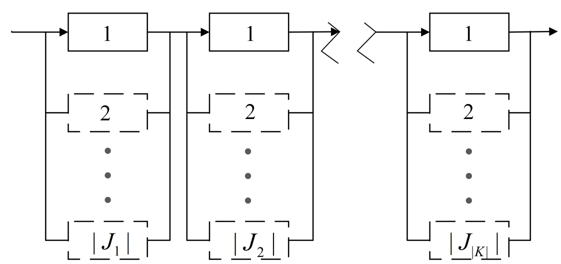
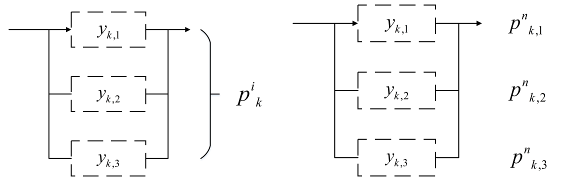


Figure 3. A serial system

This paper proposes a multi-objective optimization model that makes design decisions regarding the installation of each of the potential parallel units in order to maximize system availability and minimize total cost. For each stage k, one available unit is needed for the stage to be available. The model is solved as an ϵ-constraint optimization problem that maximizes the availability with a parametrically varied upper bound of the total cost, and yields a set of Pareto-optimal solutions. It is also shown that the original non-convex MINLP can be reformulated as an MINLP with linear constraints and a convex objective function.



(a) Stage with identical redundancies (b) Stage with non-identical redundancies

Figure 4. Sample diagrams for single stages

Multi-objective optimization problem (P1)

In this section, we present the constraints of the multi-objective optimization problem (P1) and the ϵ-constraint optimization problem (P1') that generates Pareto optimal solutions.

Defining $y_{k,j}$ as the binary variable that indicates the installation of unit j in stage k, constraint (1) states that for each stage at least one unit 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.

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

All possible scenarios are enumerated to evaluate the availability P_k of the stage, where p_k^i is the availability of the units in stage $k \in K_{iden}$ (see Figure 4(a)).

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

For stage $k \in K_{non}$ with non-identical redundancies, the availability is represented by subtracting the probabilities of unavailable scenarios(Rudd, 1962), assuming that $p_{k,j}^n$ stands for the availability of unit j in stage $k \in K_{non}$.

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

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

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

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.

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

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

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

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

As stated above, problem (P1) maximizes system availability (9) and minimizes total cost (10) subject to constraints (1) $-$ (8):

$$\max A \tag{9}$$

$$\min C^{tot} \tag{10}$$

Note that (P1) is non-convex due to constraints (4) and (5). The bi-criterion optimization problem (P1)((1)$-$(10)) is solved with the ϵ-constraint optimization problem (P1')((1)$-$(9) and (11)), which maximizes system availability (5) subject to the upper bound of total cost as shown in equation (11). The upper bound is varied parametrically to generate the Pareto-optimal curve.

$$C^{tot} \leq \cos t\_bar \tag{11}$$

Convexified formulation

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) we propose to linearize constraint (4) in order to convexify the problem by expanding the products over linear terms in (4) as summations over multi-linear terms, and then linearize them. 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: S stands for subsets of J_k; $\mathbb{S}_k$ is 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 $S = \{1,2\}$, $\alpha_{1,S} = 1, \alpha_{2,S} = 1, \alpha_{3,S} = 0$. The following equation is used to generate the subsets.

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

Here $\alpha_{j,S}$ is the digit on the jth place of the binary form of $m_S - 1$.
The binary variables $z_{k,S}$ are defined based on the sets and parameters described above:

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

Following from the definition of $z_{k,S}$, we have,

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

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

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

$$z_{k,S} \leq y_{k,j}, \quad k \in K_{non}, j \in S, S \in \mathbb{S}_k, S \neq \varnothing \tag{12}$$

$$z_{k,S} \geq \sum_{j \in S} y_{k,j} - |S| + 1, \quad k \in K_{non}, S \in \mathbb{S}_k \tag{13}$$

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:

$$\begin{aligned} P_k &= 1 - \prod_{j \in J_k} (1 - p^n_{k,j} y_{k,j}), \quad k \in K_{non} \\ &= 1 - \sum_{S \in \mathbb{S}_k} \Big(\prod_{j \in S} (-p^n_{k,j} y_{k,j})\Big)\Big(\prod_{j \in J_k \setminus S} 1\Big), \quad k \in K_{non} \\ &= 1 - \sum_{S \in \mathbb{S}_k} \Big(\prod_{j \in S} (y_{k,j})\Big)\Big(\prod_{j \in S} -p^n_{k,j}\Big), \quad k \in K_{non} \\ &= 1 - \sum_{S \in \mathbb{S}_k} z_{k,S} \prod_{j \in S} (-p^n_{k,j}), \quad k \in K_{non} \end{aligned} \tag{14}$$

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

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

Thus, the expression of $P_k, k \in K$ are all linear in (P1'L). On the other hand, let

$$A' = lnA = ln(\prod_{k \in K} P_k) = \sum_{k \in K} lnP_k \tag{15}$$

Since logarithmic functions are monotone, maximizing A' is equivalent to maximizing A. Therefore, the original objective function (9) can be replaced by (16):

$$maxA' = \sum_{k \in K} lnP_k \tag{16}$$

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 (11)–(16)) is a convex MINLP (i.e. the relaxed NLP is convex).

Illustrative examples

In this section, we illustrate the applications of the proposed model on a serial system that has 4 stages and 3 potential units for each stage displayed in Figure 5 with their corresponding availabilities. 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. (P1) is applied and solved by reformulating into its ϵ- constrained model (P1'), a non-convex MINLP. It is then reformulated as the convex MINLP (P1'L). The model is implemented in GAMS 24.4.1 on an Intel® Core™ i7, 2.93GHz. Commercial solvers BARON 14.4.0, SCIP 3.2, DICOPT(based on CONOPT 3.16D and CPLEX 12.6.1.0) and SBB 24.7.3 were used.

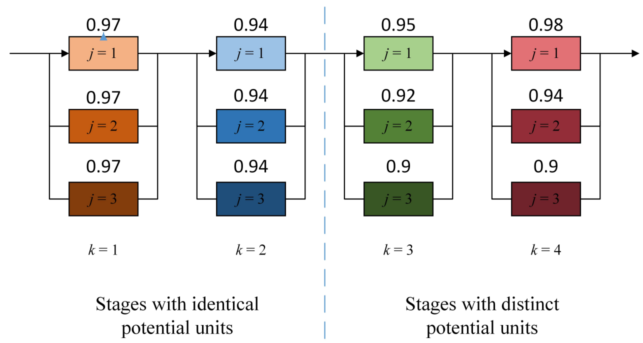


Figure 5. Case study

Table 1. Installation cost

Installation cost (k$)

	1	2	3
1		50	
2		40	
3	80	70	65
4	150	120	90

The two MINLP models are 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

Table 2. Repair cost

Repair cost (k$)			
	1	2	3
1	20		
2	4		
3	30	28	26
4	60	48	44

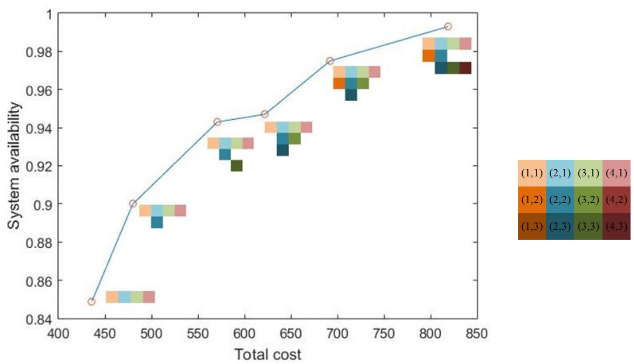


Figure 6. Pareto curve

(P1') and their linearized version, the convex MINLP's (P1'L) are identical, which are shown in Figure 6. Since the design decisions are discrete, the calculated values of C^{tot} might be less than the limit value.

In Figure 6, the small charts next to each data point indicates the design decisions in refer to the legend. As the upper bound of the cost increases, the maximum system availability increases. Figure (6) shows that the optimal designs for larger budgets usually have more units, ranging from 4 to 9. 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 discrete changes in system configuration. Table 3 compares the computational results of single models (P1') and (P1'L).

Table 3. Computational results of (P1') and (P1'L)

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

If we duplicate the stages with non-identical units by six times and consider the expanded system (example 1') with 14 stages in total, the computational results are as shown in Table 4.

Clearly, the size of problem (P1'L) is larger than that of (P1'), and the solution time of (P1'L) on example 1 is longer than that of (P1'). However, the solution time of (P1'L) on example 1' using DICOPT is shorter than that of (P1') on BARON and SCIP, which proves that the convexity of (P1'L) brings in time efficiency that should become more significant for larger problems.

Table 4. Computational results of (P1') and (P1'L) for example 1'

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

Conclusion

Assuming units with fixed availabilities, the multi-objective optimization model (P1) has been presented for selecting designs in serial systems to maximize the system availability while minimizing the cost. (P1) is solved with the non-convex MINLP model (P1'), which maximizes system availability with the total cost constrained. The convexified version of (P1'), (P1'L) is obtained through exact linearizations and redefining the objective function as the maximization of a concave function. (P1') and (P1'L) are verified to have the same optimal solutions. The Pareto curve for an illustrative example is shown and discussed.

Nomenclature

Indices

k	Stage
j	Parallel unit, smaller j has priority over larger j
l	Dummy variable for j
S	Subset of J_k

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

Parameter

n_k	Number of potential parallel units in stage k
p_k^i	Availability of single units in stage k with identical parallel units

$p^n_{k,j}$	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
$cost\_bar$	Upper bound of total cost

Variables

$y_{k,j}$	Binary variable that indicates whether unit j of stage k is selected
$z_{k,j,S}$	Binary variable that is used to convexify multi-linear terms of $y_{k,j}$
P_k	Availability of stage k
A	Availability of the entire system
C_k	Total cost for stage k
C^{tot}	Total cost of system

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