Integrating Stochastic Programming and Reliability in the Optimal Synthesis of Chemical Processes

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Abstract

Plant availability and operating uncertainties are critical considerations for the design and operation of chemical processes as they directly impact service level and economic performance. This paper proposes a two-stage stochastic programming GDP (Generalized Disjunctive Programming) model with reliability constraints to deal with both the exogenous and endogenous uncertainties in process synthesis, where the reliability model is incorporated into the flowsheet superstructure optimization. The proposed stochastic programming model anticipates the market uncertainties through scenarios for selecting the optimal flowsheet topology, equipment sizes and operating conditions, while considering the impact of selecting parallel units for improving plant availability. An improved logic-based outer-approximation algorithm is applied to solve the resulting hybrid GDP model, which effectively avoids numerical difficulties with zero flows and provides high quality design solutions. The applicability of the proposed modeling framework and the efficiency of solution strategy are illustrated with two industrial case studies: methanol synthesis process and toluene hydrodealkylation process. The model, which integrates reliability (endogenous uncertainty) and exogenous uncertainty, shows the best economic performance with the increasing operational flexibility and plant availability.

Keywords: reliability-based superstructure optimization, stochastic programming, endogenous and exogenous uncertainties, logic-based outer approximation algorithm

1. Introduction

Process synthesis is the assembly and interconnection of units into a process network, involving different physical and chemical phenomena to transform raw material and energy inputs into desired products with the goal of optimizing a given objective function (Chen & Grossmann, 2017). The superstructure-based process synthesis includes discrete variables to determine the flowsheet topology and continuous variables to determine system states. Mixed-Integer Nonlinear Programming (MINLP) and Generalized Disjunctive Programming (GDP) are two powerful modeling tools to translate the superstructure into a mathematical model that captures the logical structure of a design problem (Mencarelli et al., 2020). Both of them are well-suited to describe the problems, which involves selection among discrete process alternatives with nonlinear process phenomena (Grossmann & Trespalacios, 2013). However, the GDP formulation offers two major advantages over the traditional MINLP modeling approach in process synthesis problems. First, it is an intuitive modeling framework to explicitly express the logical-OR (disjunctive) relationship between different process alternatives, while capturing the connection between these logical clauses and the algebraic relations that describe each alternative (Chen & Grossmann, 2019). Therefore, it has a more systematic structure to formulate the grouping of related constraints in disjunctions (Raman & Grossmann, 1991). Second, GDP modeling preserves logical structure for tailored logic-based decomposition algorithms, such as logic-based outer approximation (LOA) and logic-based branch and bound algorithm (LBB), which can effectively avoid zero-flow numerical difficulties present in MINLP formulations and provide high quality design solutions (Lee & Grossmann, 2003; Ruiz & Grossmann, 2017; Türkay & Grossmann, 1996). With GDP, decomposition can be applied directly on the logical layer. These advanced solution algorithms are particularly advantageous for process synthesis problems, due to their ability to solve nonlinear subproblems in reduced space, avoid zero-flow singularities through inactive process units, thereby improving convergence speed and robustness. The extension of LOA for rigorous global optimization is also available in Pyomo.GDP via the GDPopt solver (Bergamini et al., 2005; Chen et al., 2020; Chen et al.; Trespalacios & Grossmann, 2016).

Synthesis of process flowsheets are subjected to various uncertainties, which directly impact its service level and economic performance. There are two kinds of uncertainties in process synthesis: exogenous, where the uncertain parameter values are revealed independently of optimization decisions, and endogenous, where the parameter realizations are influenced by the decisions taken (Apap & Grossmann, 2017). Exogenous uncertainties correspond typically to market uncertainties, such as product demands, product prices and utility prices. For endogenous uncertainties, decisions can influence the parameter realizations by causing alteration of the probability distribution for uncertain parameters (Type-1 endogenous uncertainties), or affecting the time at which we observe these realizations (Type-2 endogenous uncertainties) (Goel & Grossmann, 2006; Pulsipher & Zavala, 2020; Tarhan et al., 2009; Zhao & You, 2019). Fig. 1 illustrates different types of uncertainties existing in process synthesis.

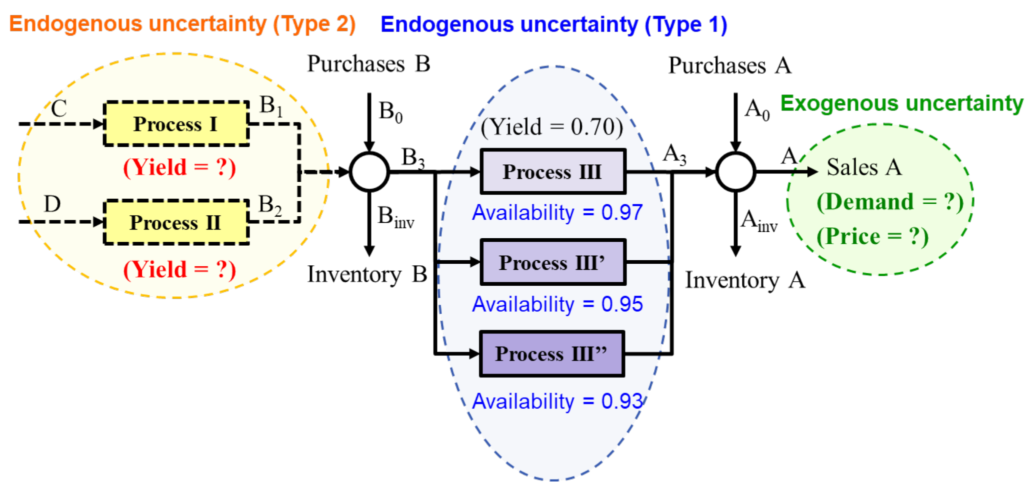

Fig.1. Classification of different types of uncertainties in process synthesis.

An example of endogenous uncertainty is reliability, which is defined as the probability that a system remains functional under component failures (Garcia-Herreros et al., 2014). The selection of redundant equipment, maintenance policy and storage sizing affect the plant availability by altering the probability distributions (Terrazas-Moreno et al., 2010; Ye et al., 2018; Ye et al., 2019). Reliability-based design optimization (RBDO) arose at the early stages for capturing the endogenous uncertainties from equipment failures, determining the topology and parameters of a system. Kuo and Wan (2007) provided a broad overview of recent research on reliability optimization problems and solution methodologies, addressing the importance of discrete decisions regarding parallel redundancies in RBDO. Aguilar et al. (2008) optimized the design and operation of flexible utility plants with reliability and availability considerations. Ye et al. (2018) proposed a rigorous non-convex MINLP model for selecting the redundant units in serial systems to optimize the availability and cost. Terrazas-Moreno et al. (2010) formulated a mixed-integer linear programming (MILP) model in the design of an integrated site subject to random failures. Design decisions which affect the availability involves increases in process capacity, introduction of parallel units, and addition of intermediate storage.

In most of the previous work, exogenous uncertainty and endogenous uncertainty (reliability) have been studied separately. Straub and Grossmann (1990) were the first contributors to provide a framework for integrating flexibility (exogenous uncertainties) and reliability (endogenous uncertainties) in a uniform framework. However, their work only considered a quantitative measure - the expected stochastic flexibility $\mathrm{E(SF)}$ that relies on discrete uncertain states to evaluate the proposed design alternatives. Thomaidis and Pistikopoulos (1994) also integrated flexibility and reliability in process design, but they did not consider the selection of standby units to improve the system availability. Therefore, there is a need to account for both types of uncertainties in process synthesis together so as to determine the feasible operation of the flowsheet to be synthesized, as well as its plant availability. In this way, the optimal design that considers the market uncertainties and inherent failures of equipment has the potential of improving the economic performance, operational flexibility and availability of process flowsheets to be synthesized.

The major goal of this paper is to propose a novel modelling framework that integrates both exogenous uncertainty through stochastic programming, and endogenous uncertainty through RBDO, for the synthesis of process flowsheets, where the reliability model is incorporated into the superstructure optimization. An improved Logic-based Outer Approximation (LOA) algorithm is applied to the resulting hybrid Generalized Disjunctive Programming (GDP) model with nested disjunctions, obtaining high-quality design solutions by avoiding zero-flow singularities.

The reminder of this article is organized as follows. The problem statement is given in Section 2. We then present the general model formulation in Section 3, followed by the solution strategy employed to tackle the resulting hybrid GDP problem in Section 4. In Section 5, two industrial cases - methanol synthesis process and toluene hydrodealkylation process, are studied to demonstrate the advantages of the proposed modeling framework and the efficiency of the solution algorithm. Finally, concluding remarks and future directions are given in Section 6.

2. Problem Statement

The general process synthesis problem that we address in this paper can be stated as follows. It is desired to transform raw material and energy inputs into desired outputs through a process network involving different physical and chemical phenomena. Given is a superstructure of all potential process alternatives, and given is a pre-specified set of potential parallel units for critical processing stages to increase the system availability. There are two types of uncertainties, which affect the service level and economic performance of the chemical process. For exogenous uncertainties, we are given a set of scenarios for uncertain demands of finished products, and uncertain prices for utility, raw material and product predicted from the changing market conditions. Each of the exogenous uncertainty is described with a discrete probability distribution captured from the historical data. For endogenous uncertainties, since critical units in the process network are subject to random failures, back-up or parallel units are given with fixed probabilities of being available. The goal is to maximize the total annualized profit of the process network by determining the optimal flowsheet structure, equipment sizes, installation of parallel units and operating conditions.

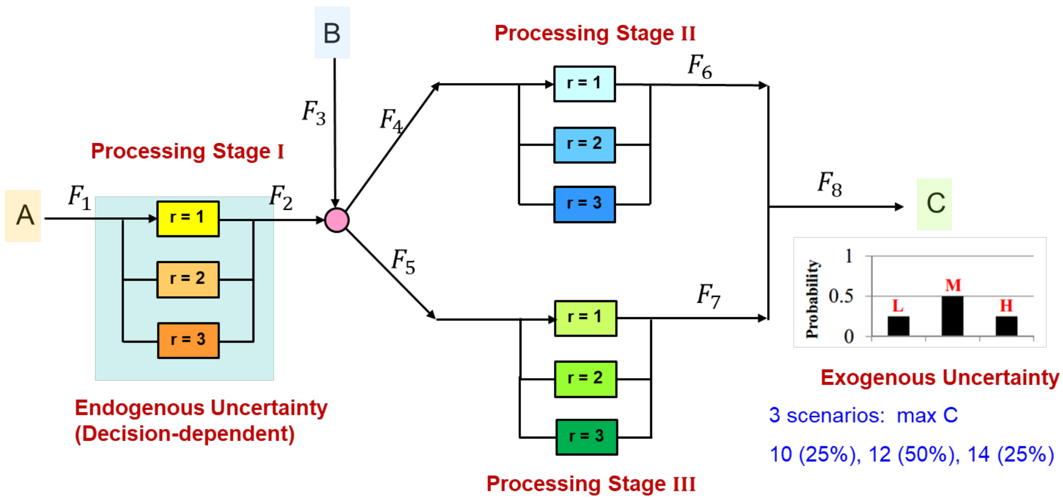

Fig. 2. Illustrative example for process synthesis with both exogenous and endogenous uncertainties taken into consideration.

3. General model formulation

The general formulation for the two-stage stochastic programming GDP model with reliability constraints is given in Problem (P1). The reliability-based design optimization (RBDO) model is incorporated into the two-stage stochastic programming to deal with both the exogenous uncertainties and endogenous uncertainties in process synthesis. The GDP model involves Boolean variables to select the optimal flowsheet topology, binary variables to decide which potential parallel units to install, and continuous variables to determine the optimal equipment sizes and operating conditions. Our goal is to determine both design- and operational-level decisions in order to maximize the total annualized profit of the system with both the exogenous uncertainties and plant availability taken into consideration.

In the proposed model (P1) below, two-stage stochastic programming is used to account for the exogenous uncertainties. The first-stage (design) decisions are made "here-and-now" before realization of any uncertainty, and the second-stage (operational) decisions are made in a "wait-and-see" manner after all the uncertainties are revealed and can be adjusted to the different scenarios as a recourse. In the process synthesis model (P1), the first-stage variables consist of three types of design variables, the Boolean variables Y_i which determine the selection among the different process alternatives, the binary variables $z_{i,r}$ to represent whether to choose the redundant unit r for the certain processing stage i and the continuous variables d_i related to the equipment sizes, such as reactor volume, number of trays in the column, surface area in the membrane separator and design capacity of heat exchanger or compressor. The second-stage decisions are related to the operational variables, such as flowrates, temperatures, and pressures. They are denoted by x_s, which are associated with each scenario s. The proposed stochastic programming model anticipates the market uncertainties through scenarios and gives multi-scenario operation strategy to increase the operational flexibility.

$$\min_{Y_i, d_i, z_{i,r}, x_s} \text{TAC} = \sum_i c_i + A_{\text{sys}} \sum_s w_s f(x_s) \qquad \text{(P1)}$$

s.t.

$$g(x_s) \leq 0, \; \forall s \in S$$

$$\begin{bmatrix} Y_i \\ h_i(d_i, x_s) \leq 0 \\ c_i = c_i^{\text{fix}} + c_i^{\text{var}} \times d_i + c_i^{\text{repa}} \end{bmatrix} \vee \begin{bmatrix} \neg Y_i \\ B^i x_s = 0 \\ c_i = 0 \end{bmatrix}, \; \forall s \in S, \; i \in I_{\bar{\text{R}}}$$

$$\begin{bmatrix} Y_i \\ h_i(d_i, x_s) \leq 0 \\ \sum_{r=1}^{n_i} z_{i,r} \geq 1 \\ z_{i,r+1} \leq z_{i,r} \quad r = 1, \dots, n_i - 1 \\ c_i = \left(c_i^{\text{fix}} + c_i^{\text{var}} \times d_i + c_i^{\text{repa}}\right) \sum_{r=1}^{n_i} z_{i,r} \\ A_i = p_i \sum_{r=1}^{n_i} z_{i,r} (1 - p_i)^{r-1} \end{bmatrix} \vee \begin{bmatrix} \neg Y_i \\ B^i x_s = 0 \\ c_i = 0 \\ A_i = 1 \end{bmatrix}, \; \forall s \in S, \; i \in I_{\text{iden}}$$

$$\begin{bmatrix} Y_i \\ h_i(d_i, x_s) \le 0 \\ \sum_{r=1}^{n_i} z_{i,r} \ge 1 \\ z_{i,r+1} \le z_{i,r} \quad r = 1, \dots, n_i - 1 \\ c_i = \sum_{r=1}^{n_i} z_{i,r}\left(\tilde{c}_{i,r}^{\text{fix}} + \tilde{c}_{i,r}^{\text{var}} \times d_i + \tilde{c}_{i,r}^{\text{repa}}\right) \\ A_i = 1 - \prod_{r=1}^{n_i}\left(1 - \tilde{p}_{i,r} z_{i,r}\right) \end{bmatrix} \vee \begin{bmatrix} \neg Y_i \\ B^i x_s = 0 \\ c_i = 0 \\ A_i = 1 \end{bmatrix}, \ \forall s \in S,\ i \in I_{\text{non}}$$

$$Y_i = \text{True} \quad \forall i \notin I_D$$

$$\Omega(Y) = \text{True}$$

$$A_{\text{sys}} = \prod\nolimits_{i \in I_{\text{iden}} \cup I_{\text{non}}} A_i$$

$$d \in R^m,\ c \ge 0,\ Y \in \{\text{True, False}\}^l,\ z \in \{0,\ 1\}^t$$

$$x_s \in R^n,\ \forall s \in S$$

Generalized Disjunctive Programming (GDP) in (P1) is applied to explicitly express the logic encapsulated in the superstructure. GDP model involves algebraic constraints, conditional constraints encapsulated within disjunctions, and logical propositions (Grossmann & Trespalacios, 2013). Here, the global constraints $g(x_s) \le 0$ describe variable relationships that must be satisfied regardless of discrete selections of the process alternatives. These include the linking constraints that equate stream flow properties between different process sections. Then the disjunctions I are posed in terms of existence or absence of units in the superstructure. Stage-1 variables $Y_i = \text{True}$ denotes the existence of a unit (processing stage), and $Y_i = False$ represents its absence. If a unit (processing stage) exists, the constraints $h_i(d_i, x_s) \le 0$ enforce for the stage-1 design variable d_i the relevant mass and energy balances, thermodynamics, kinetics, or other physical/chemical phenomena taking place within the unit for each scenario s. The constraints $c_i = c_i^{\text{fix}} + c_i^{\text{var}} \times d_i + c_i^{\text{repa}}$ calculates the total cost of the unit, including the fixed cost, the variable cost related to the equipment size and the repair cost. Otherwise, constraints $B^i x_s = 0$ describe port variable relationships when the unit is absent, and the capital cost of the non-existing unit is also set to 0.

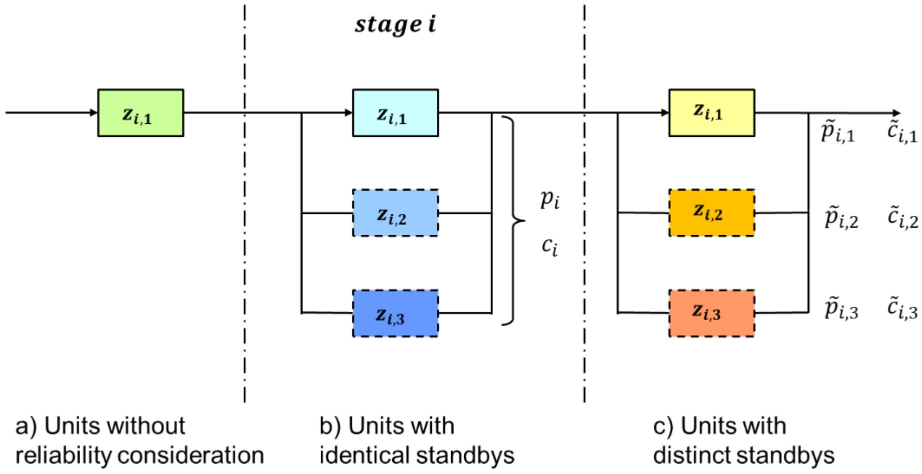

Fig.3. Sample diagram for different kinds of processing stages in process network.

The reliability-based design optimization (RBDO) model is incorporated into the GDP model to deal with the endogenous uncertainty – system availability. To integrate availability evaluations, each equipment in the flowsheet is considered as a stage, and parallel units are assigned to the certain stages i. The binary variables $z_{i,r}$, which determine the selection of the potential parallel units, affect the availability of each stage by changing the corresponding probability distribution. Each single unit is given a fixed failure rate, and Simple Bayes Rules are used to predict the system availability.

All the processing stages in the process network can be classified into three groups: the processing stages that do not need to consider the reliability $(i \in I_{\overline{\mathrm{R}}})$ because of their high capital costs and low failure rates, the stages with identical potential standby units $(i \in I_{\mathrm{iden}})$, and the stages with non-identical potential standbys $(i \in I_{\mathrm{non}})$ to improve the availability. If the processing stage i is selected, besides the mass and energy balances, physical/chemical phenomena description constraints and cost calculations, the availability evaluation model should also be added in the disjunction. For different types of processing stages, we will have the corresponding mixed-integer nonlinear constraints for reliability consideration.

For the stages with identical potential parallel units $(i \in I_{\mathrm{iden}})$, the parallel units have the same capacity, availability, and corresponding costs.

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

$$\sum_{r=1}^{n_i} z_{i,r} \geq 1 \quad i \in I \quad (1)$$

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

$$z_{i,r+1} \leq z_{i,r} \quad i \in I_{iden}, \quad r = 1, \dots, n_i - 1 \quad (2)$$

Constraint (3) calculates the availability of a certain stage i with identical parallel units. The availability of each stage is defined by the selection of potential redundant units, therefore, it can be regarded as decision-dependent endogenous uncertainty.

$$A_i = p_i \sum_{r=1}^{n_i} z_{i,r}(1-p_i)^{r-1} \quad i \in I_{iden} \quad (3)$$

The total cost of each stage with identical parallel units is then given by Constraint (4), which is the summation of fixed cost, variable cost and repair cost. It should be noted that, to deal with the bilinear terms arisen from $d_i \times z_{i,r}$, we can use exact linearization.

$$c_i = \left(c_i^{\text{fix}} + c_i^{\text{var}} \times d_i + c_i^{\text{repa}}\right) \sum_{r=1}^{n_i} z_{i,r} \quad i \in I_{iden} \quad (4)$$

For the stages with non-identical potential parallel units($i \in I_{\text{non}}$), the non-identical parallel units have the same capacities, but are distinct in terms of availability and cost.

The availability of a stage with non-identical parallel units ($i \in I_{\text{non}}$) is represented by subtracting the probabilities of all unavailable cases, as shown in Constraint (5). The availability of each stage depends on the number of installed parallel units and their respective availabilities.

$$A_i = 1 - \prod_{r=1}^{n_i} \left(1 - \tilde{p}_{i,r} z_{i,r}\right) \quad i \in I_{non} \quad (5)$$

The total cost of each stage with non-identical parallel units is given by Constraint (6).

$$c_i = \sum_{r=1}^{n_i} z_{i,r} \left(\tilde{c}_{i,r}^{\text{fix}} + \tilde{c}_{i,r}^{\text{var}} \times d_i + \tilde{c}_{i,r}^{\text{repa}}\right) \quad i \in I_{non} \quad (6)$$

Finally, the availability of the whole system is calculated from the product of the availability of each stage, as shown in Constraint (7).

$$A_{\text{sys}} = \prod\nolimits_{i \in I_{\text{iden}} \cup I_{\text{non}}} A_i \quad (7)$$

If the processing stage is not selected in the superstructure, the availability of the stage is set to 1, which will not affect the system availability. Otherwise, the availability of the stage is calculated from Simple Bayes Rules and contributes to the system availability. In addition, Y_i is set to be true when the processing unit is outside the disjunctions, which means the unit is sure to exist in the flowsheet without process alternatives.

The objective function is to minimize the total annualized cost (TAC) of the system, including the annualized capital expenditure in the first stage and the expected operating expenditure and revenue over all the scenarios in the second stage, by optimizing the flowsheet topology, equipment sizes, installation of potential parallel units and operating conditions in different scenarios. The expected revenue and operating cost are proportional to the availability of the whole system.

$$\min_{Y_i, d_i, z_{i,r}, x_s} \text{TAC} = \sum_i c_i + A_{\text{sys}} \sum_s w_s f(x_s) \quad (8)$$

4. Solution Method

When systematic superstructure-based synthesis approaches are applied to conceptual design, this generally translates to difficult mathematical programming problems with non-convex, nonlinear variable relationships. One of the most challenging characteristics of flowsheet synthesis problems for modern optimization solvers arises from "zero flow" singularities, which occur when superstructure units are absent from the flowsheet. These singularities can arise from multi-component material balances and physical property calculations in disappearing units, degrading the robustness of solution algorithms. When performance equations for these disappearing nodes (or deactivated process units) include some nonlinear functions like $\log(x)$, $x^{0.6}$, or $\frac{1}{x}$, the convergence of nonlinear solvers may suffer as a flow variable x approaches zero. The absence of flow also creates a singularity that results in degeneracy in variables that become irrelevant, such as component concentrations. Any value of the concentration is valid in the context of a solution due to the zero flow. However, these degenerate variables may participate nonlinearly in expressions that become poorly conditioned for certain variable values. The "zero-flow" numerical difficulties always exist in the chemical flowsheet synthesis problems, leading to a great barrier to most of the full-space MINLP solution algorithms that cannot eliminate constraints of non-existing process units.

The GDP formulation not only offers an intuitive way to express the logical-OR (disjunctive) relationships between different process alternatives, but also provides access to a variety of powerful logic-based decomposition algorithms that allow the robust solution of nonlinear subproblems in reduced space to avoid the zero-flow numerical difficulties. The core of LOA algorithm lies in exploiting the logical structure of a GDP model to decompose its solution into a sequence of master problems and subproblems for specific flowsheets, based on the evaluation and optimization of the full nonlinear descriptions for each logical realization. In the case of problem (P1) the subproblems correspond to MINLP subproblems that optimize the binary variables $z_{i,r}$ for determining the number of redundant units to optimize the availability.

Note that by incorporating the reliability model into the flowsheet superstructure optimization, the binary variables $z_{i,r}$ are introduced to represent the selection of parallel units. Our model becomes a hybrid GDP formulation with implicit "nested disjunctions", which not only contains the Boolean variables to select the process alternatives, but also includes binary variables to select the redundant units for improving reliability. The improved LOA algorithm for the resulting hybrid GDP model is to handle only logical realizations (Boolean variables) in the master problem, and to solve an MINLP model as the reduced space subproblem. That is, in the master problem, we still solve the linear approximation to determine a new candidate flowsheet topology (the existence of certain processing stage), but the reduced space subproblem becomes an MINLP subproblem rather than an NLP subproblem as in the original algorithm. The reduced space MINLP model corresponding to only the selected candidate flowsheet, will provides accurate equipment sizes, operating conditions, selections of parallel units and objective value. The improved logic-based outer approximation algorithm flow diagram for process synthesis problems considering reliability is described as follows and is presented in Fig. 4.

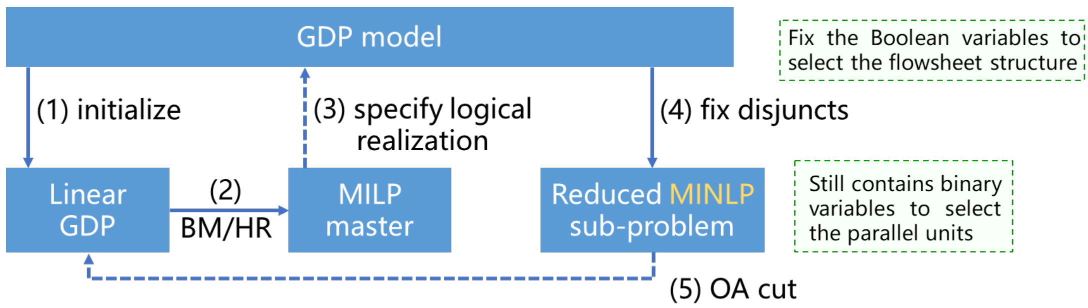

Fig.4. Improved logic-based outer approximation algorithm flow diagram for process synthesis considering reliability.

The major steps of the improved LOA algorithm (Turkay and Grossmann, 1986; Chen and Grossmann, 2019) to solve nonlinear GDP model in (P1) are as follows (See Fig. 4):

Step 1: Solve a set of MINLP subproblems to optimize different flowsheets and their parallel units in order to cover all the units in the superstructure to generate initial linearizations for the nonlinear functions in the GDP.
Step 2: Reformulate the linear GDP model to an MILP master problem through Big-M (BM) or Hull Relaxation (HR).
Step 3: Solve the MILP master problem, which yields a lower bound on the overall (minimization) problem as well as a proposed choice of the discrete variables (a candidate logical realization).
Step 4: Fix the Boolean variables in the disjunctions to the candidate logical realization calculated from the MILP master problem to obtain a reduced space MINLP subproblem.
Step 5: Solve the MINLP subproblem, which yields an upper bound on the overall (minimization) problem as well as the number of redundant units and optimal continuous variable values of the corresponding flowsheet. The solution is then used to generate an outer approximation (OA) cut.

Since the goal is to minimize the objective function, solutions obtained from the MILP master problem provide a lower bound on the remaining feasible logical realizations at each iteration (as we outer approximate the feasible region). The best feasible solution to the reduced space MINLP subproblems yields an upper bound on the objective value. Termination of the algorithm takes place when the lower bound at an iteration converges to or crosses over the upper bound, indicating that we cannot find a better solution from the set of remaining unexplored logical realizations. An infeasible master problem implies that no logical realizations remain to be explored, equivalent to a lower bound of $Z^{\mathrm{LB}} = \infty$. Convergence of LOA is checked between the master problem and reduced space subproblem solutions.

The advanced computational tool GDPopt (Chen & Grossmann, 2019), provides various implementations for solving GDP problems, including the LOA algorithm. As an open-source platform, it incorporates recent innovations in reformulation strategies and logic-based solution algorithms, which can be used as a basis of solution platform for GDP models.

5. Industrial Case Study

5.1. Methanol synthesis

5.1.1. Case Study Definition

The proposed modeling methodology and solution strategy have been applied to an industrial case study-methanol synthesis process in this section. The methanol synthesis process was formulated and solved as an MINLP model by Türkay and Grossmann (1996) without reliability and exogenous uncertainty considerations. Based on the analysis of the flowsheet superstructure, the methanol synthesis model can be converted to a hybrid GDP model with four explicit disjunctions to choose the process alternatives and several implicit "nested disjunctions" to consider the potential parallel units. Our goal is to select the optimal equipment configuration and operating conditions (temperatures, pressures, flows, and compositions) to convert syngas to methanol, with both market uncertainties and plant availability taken into consideration.

The four major structural choices in the methanol synthesis process include the discrete decisions between two candidate syngas feeds with different purity and cost, single-stage or two-stage compression for both the feed and recycle streams, as well as the choice between a higher-conversion, higher-cost reactor and a cheaper reactor alternative with low conversion. In order to incorporate the availability evaluation into the flowsheet superstructure optimization, several potential parallel units are assigned to each critical equipment, such as compressors, heat exchangers and valves. The superstructure of methanol synthesis problem with reliability consideration is shown in Figure 5. The objective is to maximize the total annualized profit for the methanol production, involving expected revenue from the methanol sales, fuel credit for the purge stream, purchase costs from the syngas feed, utility costs for the heaters and coolers, electricity costs for the compressors, and annualized capital costs for equipment purchases.

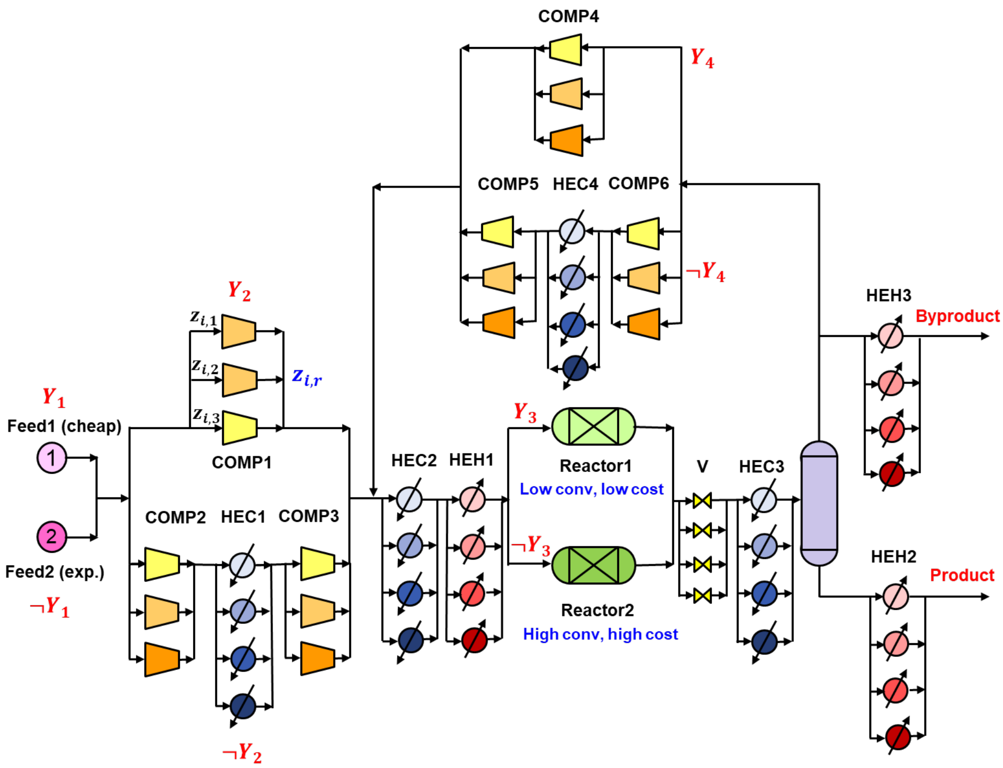

Fig.5. Superstructure of methanol synthesis problem with reliability consideration.

The synthesis of the methanol process can be formulated as a two-stage stochastic programming problem to account for the exogenous uncertainties. In the first stage the flowsheet topology and equipment configuration are selected, and in the second stage the process network operation is carried out according to the realization of uncertain parameters. In the two-stage stochastic programming, the first-stage decisions are design variables, including the Boolean variables to determine the feed selection, reactor selection, single-stage compression or two-stage compression selection, binary variables to choose the potential parallel units and continuous variables to represent the design capacity of each unit, which are related to the capital expenditure; the second-stage decisions are the operational decisions, involving flowrates, temperatures, pressures, and utility requirements, which account for the operating cost. The uncertain methanol product demand and the fluctuating electricity prices are regarded as the exogenous uncertainties. Each of them is modeled with 3 scenarios (low, medium, high demand or price) with a given discrete probability distribution, based on the historical data from the changing markets. Therefore, the two-stage stochastic programming has a total of 9 scenarios. When considering reliability, some critical units are given with fixed failure rates and parallel units are installed in these stages, the availability of the processing stage can be regarded as endogenous uncertainty. The failure of any one of these processing stages can result in the failure of the entire system, which will compromise its ability to meet customer demands and has a direct influence on the profit. The availability evaluation model is integrated within the flowsheet superstructure optimization to account for the endogenous uncertainty.

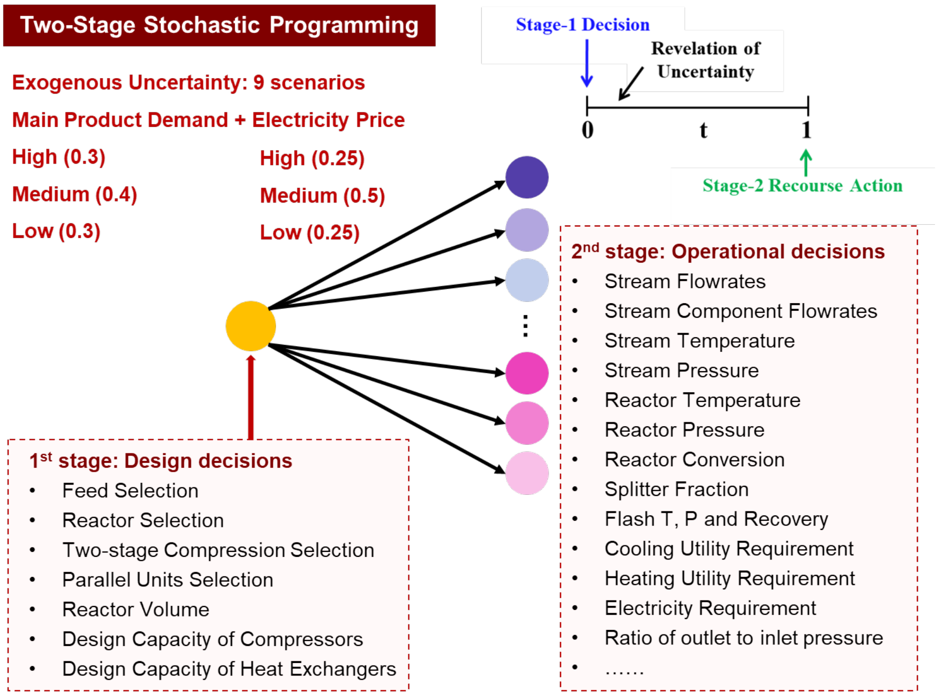

Fig.6. Two-stage representation of design- and operational-level decisions in the stochastic programming.

5.1.2. Results

Table 1. Results for different models in methanol synthesis process.

Model	# of Cons	# of Cont. Vars	# of Bin. Vars	# of Disjunctions	Strategy and Solver	Solution Time (s)	System Availability	Objective Profit (k$/yr)
Deterministic Model	474	307	0	4	LOA MILP-GUROBI NLP-CONOPT 4	35.2	0.9318	2009.16
Stochastic Programming	3986	2491	0	4	LOA MILP-GUROBI NLP-CONOPT 4	322.8	0.9318	2156.04
Integrate Reliability and Uncertainty	4306	2537	50	4	LOA MILP-GUROBI MINLP-DICOPT	446.1	0.9646	2174.96
VSS (k$/yr)	146.88				$\overline{\text{VSS}}$ (%)	7.31 %		
VSS+VRS (k$/yr)	165.80				$\overline{\text{VSS + VRS}}$ (%)	8.25 %		

To illustrate the advantages of the proposed modelling method, we compare the solution results from three different models, the deterministic model with exogenous uncertainties evaluated at their mean values, the stochastic programming model with 9 scenarios to only account for exogenous uncertainties, and our proposed model (P1) which integrates reliability and uncertainty to handle both exogenous and endogenous uncertainties simultaneously. Table 1 presents the comparison of model statistics and solution results for these three models. The first two models are standard GDP models with four disjunctions for structural choices. The last model is a hybrid GDP model (P1), which not only contains the Boolean variables to select the process alternatives, but also introduces the binary variables to select the parallel units for each critical stage. All of the three models are coded in Pyomo and solved with the LOA algorithm implemented in the GDPopt solver. All computational experiments are carried out on a PC with an Intel Core i7-6700 CPU at 2.60 GHz and 8.0 GB RAM. As aforementioned, the improved LOA algorithm involves iterative solution of the MILP master problem and the MINLP subproblem. In the first two standard GDP models, the MILP master problems are solved with GUROBI and the NLP subproblems are solved with CONOPT 4. For the proposed hybrid GDP model (P1) to integrate reliability and uncertainty, DICOPT is used to solve the MINLP subproblems due to the introduction of binary variables for reliability consideration.

In order to compare and analyse these models more scientifically, the value of stochastic solution (VSS) is calculated to evaluate the profit that can be expected from implementing the stochastic solution instead simply using the deterministic solution. Here, the VSS and relative VSS are defined in Eq. (9) and Eq. (10) respectively.

$$\mathrm{VSS} = \mathrm{Profit}^{\mathrm{sto}} - \mathrm{Profit}^{\mathrm{det}} \tag{9}$$

$$\overline{\mathrm{VSS}} = \frac{\mathrm{Profit}^{\mathrm{sto}} - \mathrm{Profit}^{\mathrm{det}}}{\mathrm{Profit}^{\mathrm{det}}} \tag{10}$$

where $\mathrm{Profit}^{\mathrm{sto}}$ is the total annualized profit calculated from the two-stage stochastic programming with the consideration of exogenous uncertainties. $\mathrm{Profit}^{\mathrm{det}}$ is obtained by solving the same stochastic problem with the first-stage variables fixed to the values at the optimal solution of the deterministic approach. That means the flowsheet structure and equipment configuration obtained from the deterministic model is also evaluated in the changing exogenous environment. VSS represents the annualized added value gained from the stochastic solution compared to the deterministic solution. Similar to the VSS, we also define the value of reliable solution (VRS) to assess the real benefits from implementing the reliability-based design optimization model and indicate the significance of accounting for endogenous uncertainty. That is, the optimal solution of the deterministic model should be evaluated with units given fixed inherent failure rates, but without the installation of parallel units to improve their availabilities. Here, the VRS and relative VRS are defined in Eq. (9) and Eq. (10) with reference to the VSS and relative VSS.

$$\mathrm{VRS} = \mathrm{Profit}^{\mathrm{reli}} - \mathrm{Profit}^{\mathrm{det}} \tag{11}$$

$$\overline{\mathrm{VRS}} = \frac{\mathrm{Profit}^{\mathrm{reli}} - \mathrm{Profit}^{\mathrm{det}}}{\mathrm{Profit}^{\mathrm{det}}} \tag{12}$$

VRS expresses the extra profit that can be expected from implementing the reliability-based design optimization model which incorporates into the superstructure optimization compared with the solution from deterministic model without reliability consideration.

Comparing the results between the deterministic model and stochastic programming model, it can be seen that the stochastic programming model to consider exogenous uncertainties shows better economic performance, with an increase of 7.31% in the total annualized profit. Significant VSS can be observed between the deterministic and stochastic solutions and the annualized additional profit of $146880 can be achieved when implementing the stochastic optimization. It is because the stochastic programming model can make adjustments to the realization of different demand and price scenarios and efficiently improve the operational flexibility. The multi-scenario operation strategy can respond to the changing markets and greatly reduce the expected operating expenditure.

Moreover, as reported in Table 1, the model that integrates reliability and uncertainty yields the best economic performance compared to the cases when either reliability is not considered, or when exogenous uncertainties are evaluated with mean values. The system availability is increased from 0.9381 to 0.9646 by adding parallel units, while the total annualized profit is increased by 8.25 % with improved operational flexibility and reliability compared to the deterministic model.

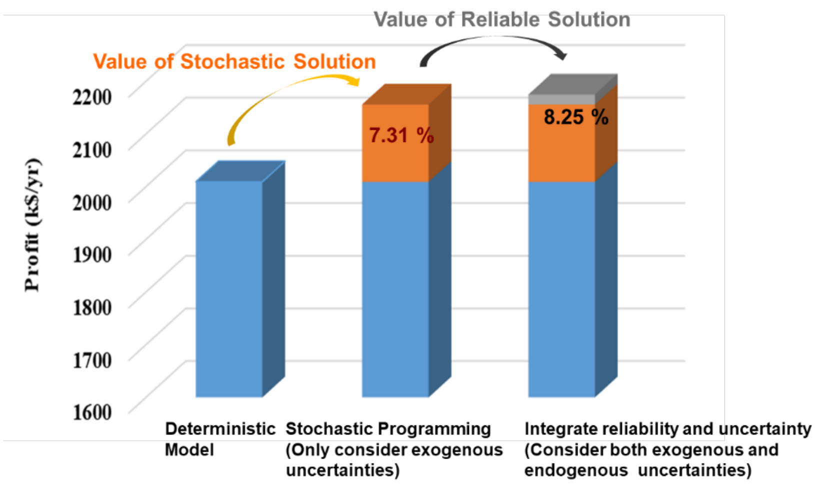

Fig. 7. Comparison of the total annualized profit for three different optimization models in terms of VSS and VRS (Methanol synthesis process).

Comparison of the total annualized profit for the three different optimization models in terms of VSS and VRS is given in Fig. 7. The orange portion represents the VSS, which means the extra profit that can be gained from implementing stochastic programming to consider exogenous uncertainties. The grey portion in the bar chart indicates the VRS, which means the extra benefit obtained from reliability-based design optimization model to account for endogenous uncertainties. The summation of the VSS and VRS means the annualized extra profit of $ 165800 can be achieved when considering both exogenous and endogenous uncertainties in the methanol process synthesis problem.

The optimal designs obtained from these three models are presented in Fig. 8-10.

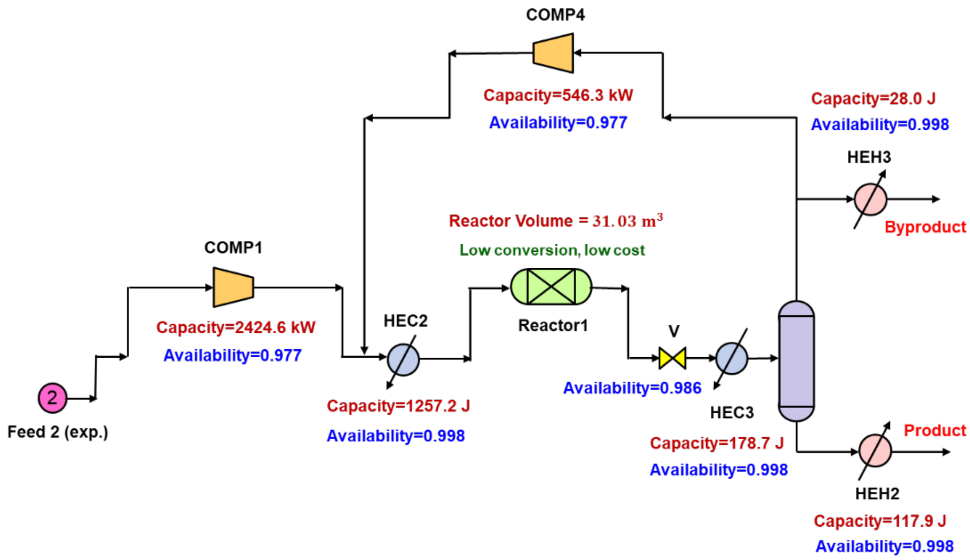

Fig. 8. Optimal design of methanol synthesis process from the deterministic model.

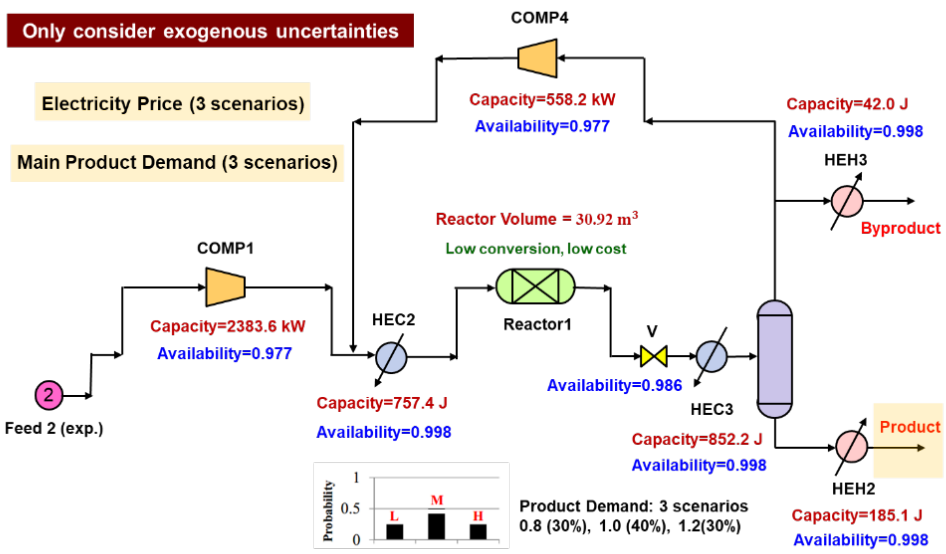

Fig. 9. Optimal design of methanol synthesis process from the stochastic programming model only to consider exogenous uncertainties.

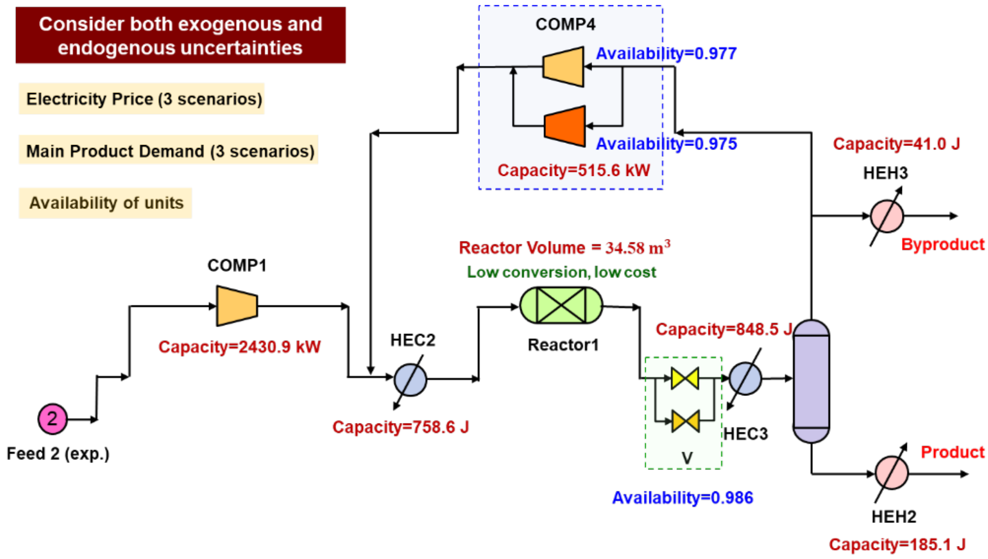

Fig. 10. Optimal design of methanol synthesis process from the integrating reliability and uncertainty model (P1).

It is interesting to note that the deterministic model and stochastic programming model have selected the same flowsheet structure, but differ in the design capacity of each unit. The differences in the design capacity make the stochastic model have a higher degree of operational flexibility, which can response to different utility price and demand scenarios and reduce the operating cost. When considering reliability, the valve and the single-stage compressor in the recycle stream both have back-up equipment in order to maximize the total annualized profit through the optimal trade-off between the capital cost and system availability.

5.2. Hydrodealkylation of toluene (HDA)

5.2.1. Case Study Definition

In this section, another industrial case study is presented to show the benefit from incorporating both exogenous uncertainties and endogenous uncertainties into the flowsheet superstructure optimization. The large-scale process synthesis problem of hydrodealkylation of toluene (HDA) process to produce benzene was formulated as an MINLP model by Kocis and Grossmann (1989) without reliability and exogenous uncertainty considerations. The superstructure of this problem is shown in Fig. 11. The objective is to maximize the total annualized profit by optimizing the flowsheet structure and operating conditions. The main reaction taken place in the HDA process is $Toluene + H_2 \rightarrow Benzene + CH_2$, with an undesired reversible side reaction $2Benzene \rightleftharpoons diphenyl + H_2$. The HDA process involves four major operations: inlet purify and mixing section, reaction system, vapor recovery system (hydrogen recycle system) and liquid separation system.

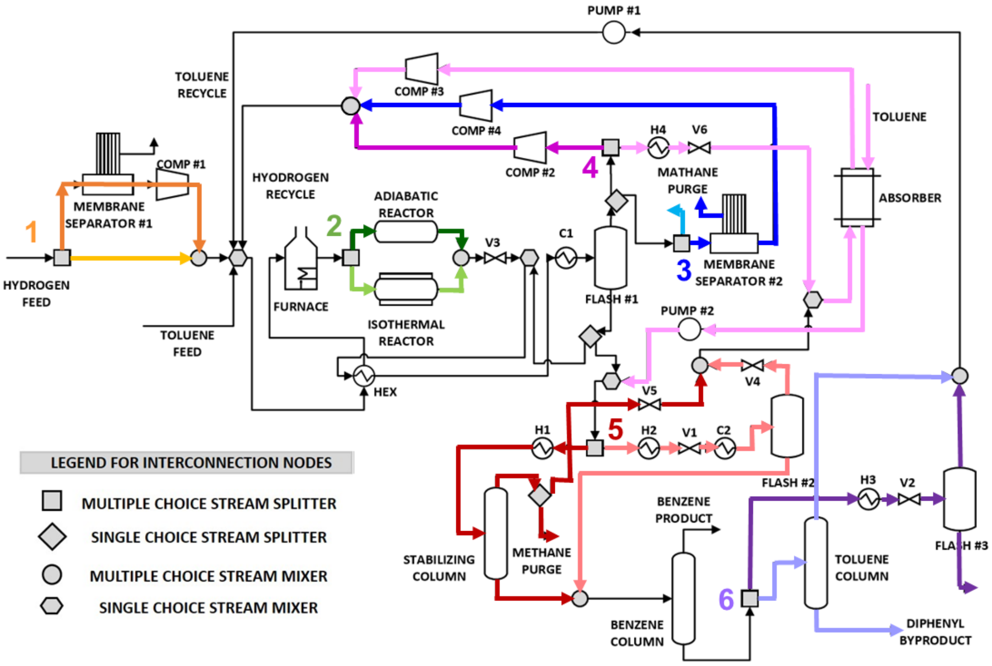

Fig. 11. Superstructure of HDA process.

To apply our proposed modeling approach, first of all, we need to convert the MINLP model into the GDP formulation. It should be noted that, between each multiple choice stream splitter and its corresponding multiple stream mixer, there will be the disjunction to represent the selection among different process alternatives. There are six multiple choice stream splitters in the superstructure, thus it has six structural choices, as shown in Fig.11, which is also described in the GDP formulation (P2) with six explicit disjunctions.

$$\begin{bmatrix} Y^{\text{membrane}} \\ \text{use membrane 1} \\ \text{use compressor 1} \\ T_{\text{inlet}}^{\text{out}} = T_{\text{membrane}}^{\text{in}} \\ P_{\text{inlet}}^{\text{out}} = P_{\text{membrane}}^{\text{in}} \\ F_{\text{bypass}} = 0 \end{bmatrix} \vee \begin{bmatrix} \neg Y^{\text{membrane}} \\ T_{\text{inlet}}^{\text{out}} = T_{\text{bypass}}^{\text{in}} \\ P_{\text{inlet}}^{\text{out}} = P_{\text{bypass}}^{\text{in}} \\ F_{\text{membrane}} = 0 \end{bmatrix} \qquad \text{(P2.1)}$$

$$\begin{bmatrix} Y^{\text{adiabatic}} \\ \text{use adiabatic reactor} \\ T_{\text{furnace}}^{\text{out}} = T_{\text{adiabatic}}^{\text{in}} \\ P_{\text{furnace}}^{\text{out}} = P_{\text{adiabatic}}^{\text{in}} \\ F_{\text{isothermal}} = 0 \end{bmatrix} \vee \begin{bmatrix} Y^{\text{isothermal}} \\ \text{use isothermal reactor} \\ T_{\text{furnace}}^{\text{out}} = T_{\text{isothermal}}^{\text{in}} \\ P_{\text{furnace}}^{\text{out}} = P_{\text{isothermal}}^{\text{in}} \\ F_{\text{adiabatic}} = 0 \end{bmatrix} \qquad \text{(P2.2)}$$

$$\begin{bmatrix} Y^{\text{methane purge}} \\ F_{\text{methane membrane}} = 0 \end{bmatrix} \vee \begin{bmatrix} \neg Y^{\text{methane purge}} \\ \text{use membrane 2} \\ \text{use compressor 4} \\ F_{\text{methane purge}} = 0 \end{bmatrix} \qquad \text{(P2.3)}$$

$$\begin{bmatrix} Y^{\text{recycle}} \\ \text{use compressor 2} \\ F_{\text{absorber}} = 0 \end{bmatrix} \vee \begin{bmatrix} \neg Y^{\text{recycle}} \\ \text{use heater 4} \\ \text{use valve 6} \\ \text{use absorber} \\ \text{use compressor 3} \\ \text{use pump 2} \\ \text{use multi splitter 4} \\ F_{\text{recycle}} = 0 \end{bmatrix} \quad \text{(P2.4)}$$

$$\begin{bmatrix} Y^{\text{stabilizing column}} \\ \text{use heater 1} \\ \text{use stabilizing column} \\ \text{use multi splitter 3} \\ \text{use valve 5} \\ T^{\text{out}}_{\text{stabilizing column}} = T^{\text{in}}_{\text{benzene column}} \\ P^{\text{out}}_{\text{stabilizing column}} = P^{\text{in}}_{\text{benzene column}} \\ T^{\text{out}}_{\text{valve 5}} = T^{\text{in}}_{\text{absorber}} \\ P^{\text{out}}_{\text{valve 5}} = P^{\text{in}}_{\text{absorber}} \\ F_{\text{flash 2}} = 0 \end{bmatrix} \vee \begin{bmatrix} \neg Y^{stabilizing\ column} \\ \text{use heater 2} \\ \text{use valve 1} \\ \text{use cooler 2} \\ \text{use flash 2} \\ \text{use valve 4} \\ T^{\text{out}}_{\text{flash 2}} = T^{\text{in}}_{\text{benzene column}} \\ P^{\text{out}}_{\text{flash 2}} = P^{\text{in}}_{\text{benzene column}} \\ T^{\text{out}}_{\text{valve 4}} = T^{\text{in}}_{\text{absorber}} \\ P^{\text{out}}_{\text{valve 4}} = P^{\text{in}}_{\text{absorber}} \\ F_{\text{stabilizing column}} = 0 \end{bmatrix} \quad \text{(P2.5)}$$

$$\begin{bmatrix} Y^{\text{toluene column}} \\ \text{use toluene column} \\ T^{\text{out}}_{\text{benzene column}} = T^{\text{in}}_{\text{toluene column}} \\ P^{\text{out}}_{\text{benzene column}} = P^{\text{in}}_{\text{toluene column}} \\ F_{\text{toluene flash}} = 0 \end{bmatrix} \vee \begin{bmatrix} Y^{\text{toluene flash}} \\ \text{use heater 3} \\ \text{use valve 2} \\ \text{use flash 3} \\ T^{\text{out}}_{\text{benzene column}} = T^{\text{in}}_{\text{heater 3}} \\ P^{\text{out}}_{\text{benzene column}} = P^{\text{in}}_{\text{heater 3}} \\ F_{\text{toluene column}} = 0 \end{bmatrix} \quad \text{(P2.6)}$$

To apply availability evaluation, several candidate parallel units are assigned to each critical equipment with reliability consideration, such as compressors, heat exchangers, pumps and valves. The equivalent reliability superstructure has 19 potential stages, with each of them having 3 potential parallel units given fixed failure rates. Exogenous uncertainties are also considered in the model, the fluctuating electricity prices and uncertain benzene demand are modeled with 3 scenarios (low, medium, high price or demand) respectively with certain discrete probability distribution. The objective function is to maximize the total annualized profit, which is given as the difference between annualized revenue and annualized cost. Revenue involves the expected sales of benzene (main product), diphenyl (by-product) and fuel values from purge streams. Costs includes the expected raw material costs, utility costs (electricity, steam, cooling water) and the investment costs for equipment and its parallel units. In the two-stage stochastic programming, the first-stages contains the selection of different process alternatives, the design capacity for each unit and the installation of parallel units. The second-stage variables are operational variables, which can be adjusted to different scenarios.

5.2.2. *Results*

Table 2. Results for different models in the HDA process.

Model	# of Cons	# of Cont. Vars	# of Bin. Vars	# of Disjunctions	Strategy and Solver	Solution Time (s)	System Availability	Objective Profit (k$/yr)
Deterministic Model	728	709	0	6	LOA MILP-GUROBI NLP-CONOPT 4	180.76	0.8253	4975.27
Stochastic Programming	2194	2110	0	6	LOA MILP-GUROBI NLP-CONOPT 4	385.52	0.8253	5194.52
Integrate Reliability and Uncertainty	2296	2252	57	6	LOA MILP-GUROBI MINLP-DICOPT	465.34	0.9993	5782.56
VSS (k$/yr)	219.25				$\overline{\text{VSS}}$ (%)	4.41 %		
VSS+VRS (k$/yr)	807.29				$\overline{\text{VSS + VRS}}$ (%)	16.2 %		

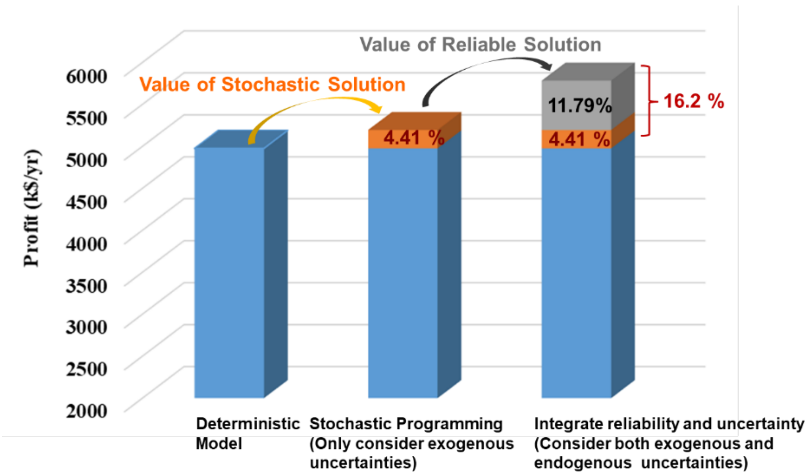

Fig. 12. Comparison of the total annualized profit for three different optimization models in terms of VSS and VRS (HDA process).

Table 2 and Figure 12 present the comparison of model statistics and solution results for the three models: 1) the deterministic model with exogenous uncertainties evaluated at their mean values, 2) the stochastic programming model with 9 scenarios to account for exogenous uncertainties, and 3) the proposed model (P1) which integrates reliability and exogenous uncertainties. The improved LOA algorithm is applied to solve these three models, where GUROBI is used to solve the MILP master problems, CONOPT 4 is used to solve the NLP subproblems and DICOPT is used to solve the MINLP subproblems when considering reliability. The VSS and VRS are calculated to evaluate the extra profit that can be expected from implementing the stochastic programming or reliability-based design optimization model instead of simply using the deterministic solution.

It can be observed that the model 3) that integrates reliability and exogenous uncertainties yields the highest total annualized profit, with an increase of 11.79% compared to the stochastic model without reliability consideration in terms of VRS, and an increase of 16.2% compared to the case with deterministic solutions in terms of VSS and VRS.

When considering reliability, the system availability increases from 0.8253 to a significantly high value 0.9993 by adding parallel units. The endogenous uncertainty plays an important part in the profit, because a penalty cost is imposed for not meeting the product demand due to the system failure.

Figures 13-15 present the optimal designs of the corresponding process flowsheets obtained from these three models.

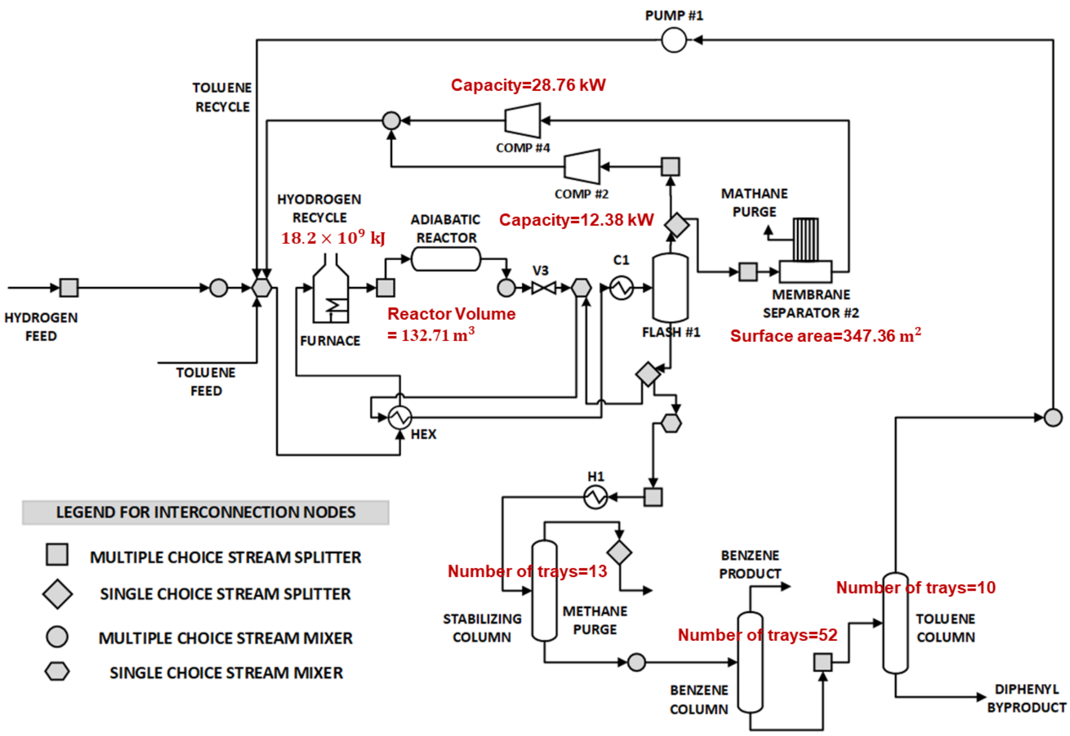

Fig. 13. Optimal design of HDA process from the deterministic model.

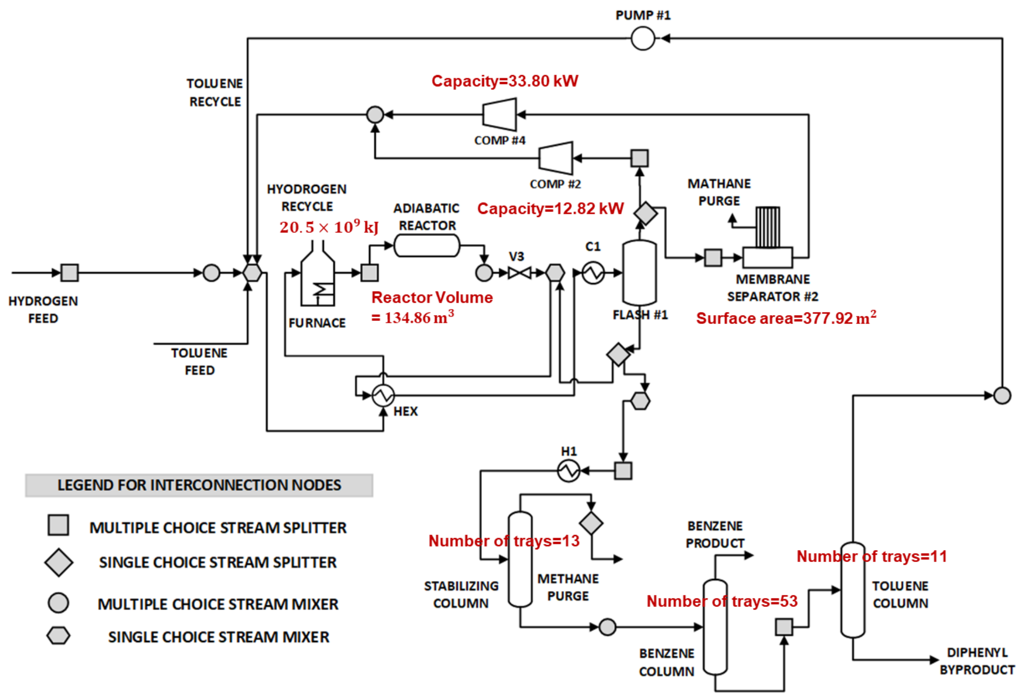

Fig. 14. Optimal design of HDA process from the stochastic programming model only to consider exogenous uncertainties.

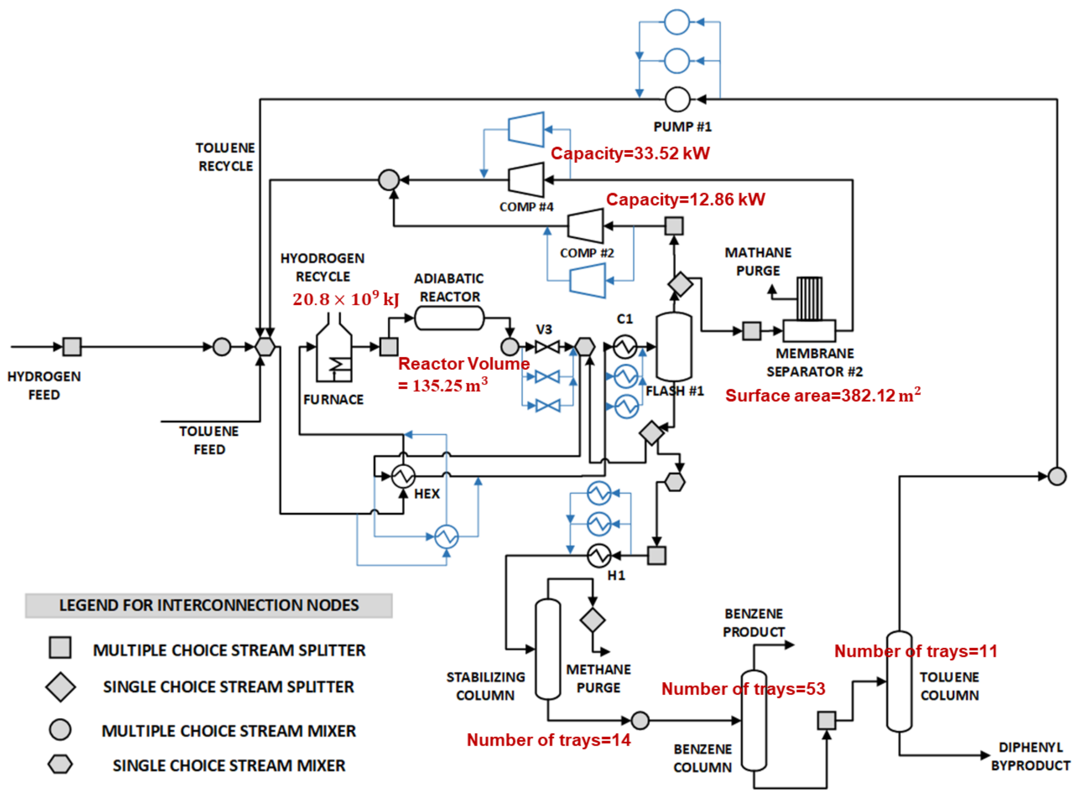

Fig. 15. Optimal design of HDA process from the integrating reliability and uncertainty model (P1).

6. Conclusions

In this paper we have addressed the optimal synthesis of process flowsheets that leads to flexible and reliable systems capable of meeting product demand and process energy requirements under various uncertainties (e.g. varying prices, demands, or equipment failures). More specifically, in this paper, we have proposed a two-stage stochastic programming GDP model with reliability constraints to deal with both the exogenous and endogenous uncertainties in process synthesis, where the reliability model is incorporated into the flowsheet superstructure optimization. We tackle the exogenous uncertainties through the two-stage stochastic programming, and account for the endogenous uncertainties by the reliability-based design optimization model, to select the optimal flowsheet topology, equipment sizes and operating conditions, as well as the installation of parallel redundant units in process synthesis. An improved LOA algorithm was developed to solve the hybrid GDP model with implicit nested disjunctions, obtaining optimal solutions by avoiding zero-flow numerical difficulties. The quantification of the value of stochastic solution (VSS) and the value of reliable solution (VRS) were used as the key measures for assessing the real benefits of the stochastic programming and reliability-based design optimization compared with the deterministic model. Simultaneous optimization of reliability (endogenous uncertainty) and exogenous uncertainty in process design provides potential improvement for operational flexibility and economic performance as shown in both the methanol synthesis and hydrodealkylation of toluene case studies.

The case studies reported in this work only have a limited number of scenarios to account for the exogenous uncertainties. However, for large-scale scenario-based stochastic programming process synthesis problems, the exponentially growing problem requires decomposition algorithms to reduce the computational effort. This will be subject of future work.

Acknowledgments

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Nomenclature

Indices

i	Stage
r	Parallel unit
s	Scenario

Sets

I	Set of processing stages (e.g. absorption)

I_{iden}	Set of stages with identical parallel units
I_{non}	Set of stages with non-identical parallel units
$I_{\bar{\text{R}}}$	Set of stages without reliability consideration
I_D	Set of stages in the disjunctions
S	Set of scenarios in the stochastic programming

Variables

Y_i	Boolean variables which determine the selection among the process alternatives
$z_{i,r}$	Binary variables that indicate whether to choose parallel unit r in stage i
d_i	Continuous variables related to the equipment sizes (which indicate the design capacity of parallel units in stage i)
x_s	Operational variables in scenario s (e.g. flowrates, temperatures and pressures)
c_i	Total cost for stage i
A_i	Availability of stage i
A_{sys}	Availability of the whole system

Parameters

n_i	Number of potential parallel units in stage i
p_i	Availability of single unit in stage i with identical parallel units
$\tilde{p}_{i,r}$	Availability of single unit r in stage i with non-identical parallel units
c_i^{fix}	Fixed cost for single unit in stage i with identical parallel units
c_i^{var}	Variable cost for single unit in stage i with identical parallel units
c_i^{repa}	Repair cost for single unit in stage i with identical parallel units
$\tilde{c}_{i,r}^{\text{fix}}$	Fixed cost for single unit r in stage i with non-identical parallel units
$\tilde{c}_{i,r}^{\text{var}}$	Variable cost for single unit r in stage i with non-identical parallel units
$\tilde{c}_{i,r}^{\text{repa}}$	Repair cost for single unit r in stage i with non-identical parallel units
w_s	Probability of occurrence of each scenario s in the stochastic programming

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