

Provided for non-commercial research and education use.  
Not for reproduction, distribution or commercial use.



This article appeared in a journal published by Elsevier. The attached copy is furnished to the author for internal non-commercial research and education use, including for instruction at the authors institution and sharing with colleagues.

Other uses, including reproduction and distribution, or selling or licensing copies, or posting to personal, institutional or third party websites are prohibited.

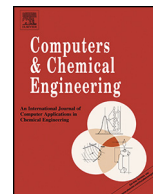
In most cases authors are permitted to post their version of the article (e.g. in Word or Tex form) to their personal website or institutional repository. Authors requiring further information regarding Elsevier's archiving and manuscript policies are encouraged to visit:

<http://www.elsevier.com/authorsrights>



Contents lists available at ScienceDirect

## Computers and Chemical Engineering

journal homepage: [www.elsevier.com/locate/compchemeng](http://www.elsevier.com/locate/compchemeng)

## Profit optimization for chemical process plant based on a probabilistic approach by incorporating material flow uncertainties

Mesfin Getu<sup>a,\*</sup>, Shuhaimi Mahadzir<sup>b</sup>, Moonyong Lee<sup>c</sup><sup>a</sup> Chemical Engineering Department, Curtin University of Technology, CDT 250, 98009 Miri, Sarawak, Malaysia<sup>b</sup> Chemical Engineering Department, Universiti Teknologi Petronas, Bandar Seri Iskandar, 31750 Tronoh, Perak, Malaysia<sup>c</sup> School of Chemical Engineering, Yeungnam University, 214-1 Dae-dong, Gyeongsan, Gyeongbuk 712-749, Republic of Korea

## ARTICLE INFO

## Article history:

Received 8 October 2012

Received in revised form 20 March 2013

Accepted 8 May 2013

Available online 18 June 2013

## Keywords:

HYSYS

GAMS

Optimization

Profit

Uncertainty

## ABSTRACT

This paper reports how the economic performance of a chemical process plant is affected by material flow uncertainties from the plant inlet and outlet. Two chance-constrained optimization models were proposed. The models were tested using case studies of an existing gas processing plant. Profit optimization for the case studies was made with respect to the reliability of holding the process constraints at a certain confidence level [0.5, 1]. The optimal profit change for uncertainty from the plant inlet within the confidence interval [0.96, 1] was 86%. On the other hand, the optimal profit change for uncertainty from the plant outlet was only 2% for the same confidence level interval considered. This suggests that the uncertainty from the plant inlet has a major impact on the overall economic performance of the plant. Sensitivity analysis showed how uncertain parameters from both plant sides can affect the overall profit significantly.

© 2013 Elsevier Ltd. All rights reserved.

## 1. Introduction

Chemical process plants normally have to consider significant uncertainties due to both internal and external factors (Ierapetritou, Acevedo, & Pistikopoulos, 1996; Li & Ierapetritou, 2008; Sahinidis, 2004). Previous studies on the uncertainty of chemical process plants focused mainly on process design where emphasis was given to the feasibility test and flexibility index (Grossmann, Halemane, & Swaney, 1983; Swaney & Grossmann, 1985a, 1985b). In addition to the design, uncertainties were also considered in process planning under demand uncertainty (Ahmed & Sahinidis, 1998; Gupta & Maranas, 2000; Petkov & Maranas, 1997). On the other hand, only a few studies focused on the uncertainty for plant operation (Arellano-Garcia, Wendt, Li, & Wozny, 2003; Arellano-Garcia & Wozny, 2009; Li, Arellano-Garcia, & Wozny, 2008; Li, Wendt, & Wozny, 2004). The uncertainty during plant operation propagates through the material and energy flows. Moreover, material flow uncertainties have a significant effect on the overall economic performance of a plant (Mesfin, Shuhaimi, & Lee, 2012). Therefore, it is important to determine how it can actually affect the plant's profit by treating the uncertainties that arise from the plant inlet and outlet sides separately.

Optimization problems are generally approached in three main directions, which can be distinguished broadly as follows: (a) deterministic programming; (b) fuzzy programming and (c) stochastic programming. In deterministic optimization, the description of uncertainty is provided either by specific bounds or a finite number of fixed parameters (Li et al., 2008). In most cases, the expected or nominal value of the uncertain parameter was used. As a result, the uncertain parameter will deviate from its expected value and the constraints may also be violated (Wendt, Li, & Wozny, 2002).

In the fuzzy optimization problem, fuzzy numbers are defined on a fuzzy set to represent the uncertain parameters in the model. In this approach, some constraint violation is allowed and the degree of satisfaction of a particular constraint is defined as membership function of the constraint (Sahinidis, 2004). Although the fuzzy programming approach provides a better solution compared to the deterministic optimization, it has still some limitations in terms of its rigorousness compared to stochastic programming (Liu & Sahinidis, 1996).

Stochastic programming consists of two approaches: two-stage programming and probabilistic or chance-constrained programming. In two-stage programming, the decision variables are divided into two sets. The first stage variables are determined before realizing the uncertain variables. The second stage variables are then used as a corrective measure against any infeasibility that may arise due to the presence of uncertainty. One of the limitations of two-stage optimization is that the number of iterations between the first and second stage variables requires more computational effort. In

\* Corresponding author. Tel.: +60 147549286; fax: +60 85443837.  
E-mail addresses: [mesfin.g@curtin.edu.my](mailto:mesfin.g@curtin.edu.my), [mesfin.getu@yahoo.com](mailto:mesfin.getu@yahoo.com), [mesfin.getu@gmail.com](mailto:mesfin.getu@gmail.com) (M. Getu).

addition, the penalty term used for compensation in the objective function is sometimes intangible and difficult to measure (Li, Hui, Li, & Li, 2004).

Probabilistic or chance-constrained programming is one of the emerging competitive tools in process system engineering, particularly for optimization under uncertainty (Li et al., 2008). In this method, the uncertain variables are held using a prescribed probability or confidence level. The method ensures not only the optimality and flexibility of the plant operation but also the reliability of holding the process constraints at a specified probability or confidence level. The performance of this approach has been compared with deterministic, worst-case and two-stage programming (Mesfin & Shuhaimi, 2010). Unlike other methods, the probabilistic/chance-constrained method has numerous advantages in providing an optimal solution by considering profit with respect to holding the process constraints at a certain probability level.

This paper presents a practical evaluation of those uncertainties that arise from the plant inlet and outlet. The uncertainties were treated separately and compared to determine their effects on the overall economic performance of the plant. Such quantitative analysis has not been reported previously. The results are expected to answer the following questions: Which uncertainty has a greater effect on the overall economic performance of the plant? For which uncertainty should more emphasis be given and under what circumstances? Which material component flow has a significant effect on the plant performance in terms of both profitability and operability? Regarding when the plant engineer wants to shift the production line, which constraints should be held to a certain confidence level so that the plant can generate high revenue?

These and other several issues will be examined in this paper. Based on this, two probabilistic optimization models were developed, where the first was for the material flow uncertainties from the plant inlet, whereas the second one for material flow uncertainties from the plant outlet. The models were tested by taking two case studies for an existing gas processing plant (GPP). The entire GPP process was initially represented using rigorous HYSYS (ASPEN HYSYS, 2006). Later, profit and sensitivity analysis was made for each of the cases by solving the developed optimization models using general algebraic modeling system or GAMS (Rosenthal, 2006).

## 2. Modeling material inflow and outflow

Any chemical process plant produces outflows by processing some inflows. These inflows and outflows consist of material and utilities. The material flow is comprised of the raw materials as feedstock and the material products produced from the plant. The utilities are steam, cooling water, refrigerant, electricity, fuel oil and others. The supply and demand of these inflows and outflows fluctuate constantly (Li et al., 2008). Moreover, the material flows have significant impact on the overall economic performance of the plant compared to the utilities. Furthermore, for the material inflows, there are continuous variations as their supply might arise from the upstream plant or sometimes from another downstream plant. For material outflow, there might be a different requirement on the product specification based on the consumer demand. Therefore, it is important to determine the economic impact of those material inflows and outflows by incorporating their uncertainty effect.

Fig. 1 presents the general representation of material inflows and outflows of a chemical process plant. The material inflows that could be decided (certain) are represented as  $R$ , whereas those that are uncertain are represented as  $\hat{R}$ . Similarly,  $P$  and  $\hat{P}$  represent the certain and uncertain material outflows, respectively. The material balance is the basic factor that determines the performance of the

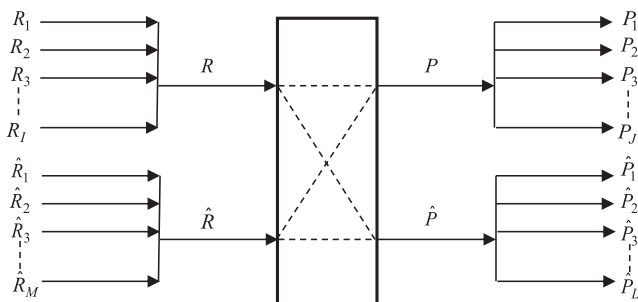


Fig. 1. Schematic diagram of the material inflows and outflows of a chemical process plant.

plant. It helps to optimize the consumption of raw material by pursuing systematically the internal flows in the production process. Li, Wendt, et al. (2004) suggested that a linear mass and energy balance is usually preferred in industrial practice to model the internal mass and energy flows. However, there are certain assumptions that could be considered during the modeling steps. The general material balance equation based on Fig. 1 can be expressed as:

$$\sum_{j=1}^J a_{k,j} P_j + \sum_{l=1}^L \hat{a}_{k,l} \hat{P}_l = \sum_{i=1}^I b_{k,i} R_i + \sum_{m=1}^M \hat{b}_{k,m} \hat{R}_m \quad (1)$$

In Eq. (1),  $a$ ,  $\hat{a}$ ,  $b$  and  $\hat{b}$  are coefficients from material inflows and outflows. The index  $k$  represents the components involved in the raw materials and products. The indices  $i$  and  $j$  represent for certain raw material and product flows, respectively.  $m$  and  $l$  are indices for uncertain raw material and product flows, respectively.

Once the formulation for the material balance is obtained, the next step is to formulate the deterministic optimization model. Developing a basic deterministic optimization model initially helps convert to the corresponding probabilistic model (Li et al., 2008).

## 3. Deterministic model formulation

The feeds entering a chemical process plant might consist of multiple streams that are combined and processed to produce the desired products, as shown in Fig. 1. The goal of deterministic optimization is to determine the decision variables that maximize or minimize some aspects of the model. The body of the optimization model consists of an objective function and constraints. In deterministic optimization, the model first simulates the flow-sheet and calculates the decision variables, objective function and constraints. The information is then utilized by the optimizer to calculate a new set of decision variables. This iterative sequence continues until the optimization criteria are satisfied (Diwaker, 2008). The objective function formulation for the deterministic optimization becomes:

$$\max \text{Profit} = \sum_{j=1}^J \bar{C}_j^P P_j - \sum_{i=1}^I \bar{C}_i^R R_i \quad (2)$$

where  $\bar{C}^R$  and  $\bar{C}^P$  are the expected price factors for certain raw material and product flows, respectively. The constraints from the plant material flows are described below:

Inlet material flow distribution to the plant:

$$R = \sum_{i=1}^I R_i \quad (3)$$

Outlet material flow distribution from the plant:

$$P = \sum_{j=1}^J P_j \quad (4)$$

Availability of material flow constraint:

$$\sum_{j=1}^J a_{k,j} P_j \leq \sum_{i=1}^I b_{k,i} R_i, \quad k = 1, \dots, K \quad (5)$$

Total material balance:

$$P = R \quad (6)$$

Material flow capacity restriction:

$$R_{i,\min} \leq R_i \leq R_{i,\max}, \quad i = 1, \dots, I \quad (7)$$

$$P_{j,\min} \leq P_j \leq P_{j,\max}, \quad j = 1, \dots, J \quad (8)$$

#### 4. Probabilistic model formulation

Once the deterministic model is developed, the next step is to formulate the corresponding probabilistic models. The probabilistic models were developed by considering the uncertainty from the plant inlet and outlet sides. The formulations of these two models are discussed as follows.

##### 4.1. Uncertainty modeling from the plant inlet

By considering the uncertainty of material flows from the plant inlet side only, Eq. (1) is reduced to:

$$\sum_{j=1}^J a_{k,j} P_j - \sum_{i=1}^I b_{k,i} R_i = \sum_{m=1}^M \hat{b}_{k,m} \hat{R}_m = r_k^\xi, \quad k = 1, \dots, K \quad (9)$$

where  $\xi_k \subseteq \mathfrak{R}^k$  is a vector of the total uncertain feed component inflows and  $r_k^\xi$  represent the total actual uncertain feed component flow rate that enter the plant. The objective function in this case is described as:

$$\max \text{Profit} = \sum_{j=1}^J \bar{C}_j^P P_j - \sum_{i=1}^I \bar{C}_i^R R_i - \bar{C}^{\hat{R}} \left[ \sum_{k=1}^K r_k^\xi \right] \quad (10)$$

In this formulation, some of the constraints from the deterministic optimization remain the same, such as Eqs. (4), (7) and (8). The new constraints introduced can be expressed as:

$$R = \sum_{i=1}^I R_i, \quad \hat{R} = \sum_{k=1}^K r_k^\xi \quad (11)$$

$$\Pr_k \left\{ r_k^\xi = \sum_{j=1}^J a_{k,j} P_j - \sum_{i=1}^I b_{k,i} R_i \leq \xi_k \right\} \geq \alpha_k, \quad k = 1, \dots, K \quad (12)$$

$$\Pr \left\{ r_k^\xi = \sum_{j=1}^J a_{k,j} P_j - \sum_{i=1}^I b_{k,i} R_i \leq \xi_k, \quad k = 1, \dots, K \right\} \geq \alpha \quad (13)$$

$$P = R + \hat{R} \quad (14)$$

where Pr is the probability operator for holding the constraints. The probabilistic constraints shown in Eqs. (12) and (13) are held at a certain user-defined probabilistic level or confidence level ( $\alpha$ ).

These types of constraints can be held in two ways. If the constraint is held individually for each  $\alpha_k$  ( $k = 1, \dots, K$ ), it is referred to as single chance constraint as described in Eq. (12). On the other hand, if the constraints are held as a whole with a common confidence level ( $\alpha$ ) for the components ( $k = 1, \dots, K$ ), the constraint is called joint chance constraint, as shown in Eq. (13).

To solve the probabilistic constraint shown in Eqs. (12) and (13), a relaxation step needs to be made to convert them to the corresponding equivalent deterministic form. The problem can then be solved using the available commercial software routines (Li et al., 2008). The relaxation step begins from the probability computation for both the single and joint chance constrained. The probability computation allows quantification of the uncertain inflows using a known probability density function. Based on this, the probability computation for independent uncertain flows  $\xi$  can be expressed as:

$$\Phi(r_k^\xi) = \Pr_k \{ \xi_k \leq r_k^\xi \} = \int_{-\infty}^{r_k^\xi} \rho_k(\xi_k) d\xi_k, \quad k = 1, \dots, K \quad (15)$$

where  $\rho$  refers to the probability density function for the uncertain variable  $\xi$ . The symbol  $\Phi$  is the probability distribution function with  $\Phi(\infty)=1$ . The equivalent deterministic form for the probabilistic constraints shown in Eqs. (12) and (13) can be expressed as Eqs. (16) and (17), respectively;

$$\sum_{j=1}^J a_{k,j} P_j - \sum_{i=1}^I b_{k,i} R_i \leq \Phi_k^{-1}(1 - \alpha_k), \quad k = 1, \dots, K \quad (16)$$

$$\prod_{k=1}^K \left[ 1 - \Phi_k \left( \sum_{j=1}^J a_{k,j} P_j - \sum_{i=1}^I b_{k,i} R_i \right) \right] \geq \alpha \quad (17)$$

where  $\Phi^{-1}$  is a parameter for the inverse value of the probability distribution function. The inverse value  $\Phi^{-1}$  is a known value at the specified confidence levels  $\alpha$ . The relaxed constraint in Eq. (16) can be solved using LP solvers, such as CPLEX. On the other hand, the relaxed joint chance constraint shown in Eq. (17) requires a NLP solver, such as CONOPT, MINOS and SNOPT.

##### 4.2. Uncertainty modeling from the plant outlet

Similarly, by considering the uncertainty from the plant outlet side only, Eq. (1) can be re-written as:

$$p_k^\zeta = \sum_{l=1}^L \hat{a}_{k,l} \hat{P}_l = \sum_{i=1}^I b_{k,i} R_i - \sum_{j=1}^J a_{k,j} P_j, \quad k = 1, \dots, K \quad (18)$$

where  $\zeta_k \subseteq \mathfrak{R}^K$  is a vector of the total actual uncertain product component outflows and  $p_k^\zeta$  represents the total uncertain product component flow rate that is produced from the plant. The objective function in this formulation can be expressed as:

$$\max \text{Profit} = \sum_{j=1}^J \bar{C}_j^P P_j + \bar{C}^{\hat{P}} \left[ \sum_{k=1}^K p_k^\zeta \right] - \sum_{i=1}^I \bar{C}_i^R R_i \quad (19)$$

where  $\bar{C}^{\hat{P}}$  is the expected price factor for the uncertain product flow. The equations that remain the same from the deterministic optimization are Eqs. (3), (7) and (8). The new constraints can be expressed as:

$$P = \sum_{j=1}^J P_j, \quad \hat{P} = \sum_{k=1}^K p_k^\zeta \quad (20)$$

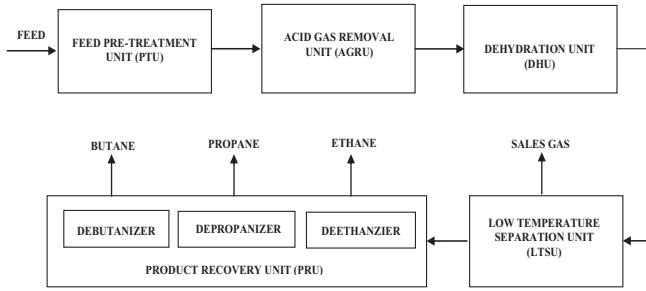


Fig. 2. Simplified block diagram for a gas processing plant (GPP).

$$Pr_k \left\{ p_k^\zeta = \sum_{i=1}^I b_{k,i} R_i - \sum_{j=1}^J a_{k,j} P_j \geq \zeta_k \right\} \geq \alpha_k, \quad k = 1, \dots, K \quad (21)$$

$$Pr \left\{ p_k^\zeta = \sum_{i=1}^I b_{k,i} R_i - \sum_{j=1}^J a_{k,j} P_j \geq \zeta_k, \quad k = 1, \dots, K \right\} \geq \alpha \quad (22)$$

$$P + \hat{P} = R \quad (23)$$

The probability computation for the independent uncertain flow  $\zeta$  is given as:

$$\Phi(p_k^\zeta) = Pr_k\{\zeta_k \leq p_k^\zeta\} = \int_{-\infty}^{p_k^\zeta} \rho k_k(\zeta_k) d\zeta_k, \quad k = 1, \dots, K \quad (24)$$

The corresponding equivalent deterministic constraints for Eqs. (21) and (22) can be written as Eqs. (25) and (26), respectively;

$$\sum_{i=1}^I b_{k,i} R_i - \sum_{j=1}^J a_{k,j} P_j \geq \Phi_k^{-1}(\alpha_k), \quad k = 1, \dots, K \quad (25)$$

$$\prod_{k=1}^K \left[ \Phi_k \left( \sum_{i=1}^I b_{k,i} R_i - \sum_{j=1}^J a_{k,j} P_j \right) \right] \geq \alpha \quad (26)$$

The optimization problems formulated in Eqs. (10)–(17) and (19)–(26) can be plotted in terms of the reliability of the process and the profitability of the plant, which will be discussed in Section 5. The reliability of a process is defined as to what extent the process can be held so that the violation of constraint is reduced to a certain level. The profitability of the plant is the corresponding economic performance of the plant at a specified reliability of the process. Therefore, the relationship between the reliability of the process and profitability of the plant can be determined by repeatedly solving the optimization problem at different confidence levels.

## 5. Case studies

A typical gas processing plant is comprised of the following main processes: (a) pre-treatment unit (PTU); (b) acid gas removal unit (AGRU); (c) de-hydration unit (DHU); (d) low temperature separation unit (LTSU); (e) sales gas compression unit (SGCU); and (f) product recovery unit (PRU). Fig. 2 shows a simplified schematic representation of a gas processing plant for the main processes and products involved. The feeds to the plant consist of seven components:  $C_1$ ,  $C_2$ ,  $C_3$ ,  $C_{4s}$ ,  $C_{5+}$ ,  $N_2$  and  $CO_2$  ( $k = 1, \dots, 7$ ). The main products produced from the plant include sales gas ( $P_1$ ), ethane ( $P_2$ ), propane ( $P_3$ ) and butane ( $P_4$ ). In addition, by-products formed from the plant include carbon dioxide ( $P_6$ ) from AGRU and condensate or heavier hydrocarbon products ( $P_5$ ) from PRU.

Table 1  
Mean and standard deviations of the uncertain feed component inflows.

Components ( $k$ )	Uncertain feed component inflows ( $\xi_k$ )	Mean (ton/h)	Standard deviation (ton/h)
$C_1$	$\xi_1$	190.0522	31.360
$C_2$	$\xi_2$	32.2608	5.788
$C_3$	$\xi_3$	20.782	4.289
$C_{4s}$	$\xi_4$	13.082	3.173
$C_{5+}$	$\xi_5$	9.060	3.348
$N_2$	$\xi_6$	2.439	0.656
$CO_2$	$\xi_7$	47.224	9.742

Table 2  
Maximum and minimum values of decision variables for uncertain feed flow case.

Raw material and products	Maximum value (ton/h)
$R_3$	10.706
$R_4$	35.586
$P_1$	298.518
$P_2$	37.311
$P_3$	47.706
$P_4$	29.586
$P_5$	43.111
$P_6$	57.659

A simulation model for the entire plant was developed using ASPEN HYSYS and the optimization models were solved using GAMS. Two case studies were performed: the first focused on the material flow uncertainty from the plant inlet, whereas the second focused on the plant outlet.

### 5.1. Case study 1

For this case study, the feed shown in Fig. 2 consists of four individual inlet streams, where  $\hat{R}_1$  and  $\hat{R}_2$  are highly uncertain as their supply originates from the upstream plant. The remaining two feed  $R_3$  and  $R_4$  are normally known and can be decided. All the products from the plant outlet are considered to be decided. The product recovery unit (PRU) consists of three conventional distillation columns, as shown in Fig. 2. The arrangement of the columns for this case study is with a deethanizer first, depropanizer second and finally a debutanizer.

#### 5.1.1. Data analysis

A large set of data for the uncertain feed flows,  $\hat{R}_1$  and  $\hat{R}_2$ , with each containing approximately 8785 data points on an hourly basis were taken and are presented in Appendix A (Figs. A1 and A2). A normal distribution was assumed based on the data distribution obtained from the plant. Table 1 lists the mean and standard deviations of the uncertain feed component inflows ( $\xi_1, \xi_2, \dots, \xi_7$ ). Table 2 presents the maximum values for the raw material and products flows, which are considered as decision variables. The minimum values were set zero for all the decision variables. Table 3

Table 3  
Expected price value for products and raw material.

Raw material and product	Expected value (\$/ton)
$\hat{R}_1$	35.631
$\hat{R}_2$	28.871
$R_3$	15.132
$R_4$	21.441
$P_1$	101.941
$P_2$	61.031
$P_3$	166.712
$P_4$	212.013
$P_5$	-
$P_6$	-



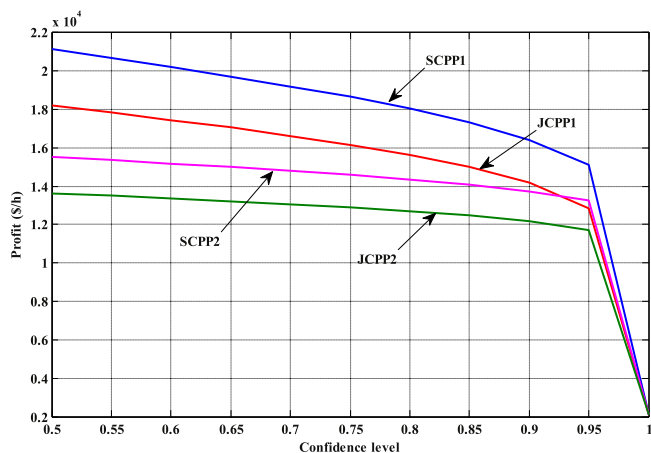


Fig. 3. Optimal profit profiles for the uncertain feed case.

shows the expected price factor for each raw material and products. The expected price factor for the condensate product was assumed to be nil because the plant currently does not generate revenue from this product.

### 5.1.2. Optimization

The optimization problem formulation for this case study begins by examining Eqs. (10) to (17). Based on this, the single and joint chance constrained optimization problem have been formulated and shown in Appendix B (Eqs. (B-1)–(B-16)). Fig. 3 presents the optimal profit profiles, SCPP1 (single chance profit profile 1) and JCPP1 (joint chance profit profile 1), beginning from the 50% to 100% confidence level. The 50% confidence level was taken as an initial evaluation based on the fact that the uncertain parameter in deterministic optimization is normally held at their average value. The evaluation at the 100% confidence level was approximated to 0.999999, which approaches unity. For SCPP1, each individual single chance constraints were held initially at the 50% confidence level, and then at the 55% confidence level with a 5% interval difference until the 100% confidence level. On the other hand, for JCPP1, all the constraints were held initially at a common 50% confidence level and later varied in 5% intervals until the 100% confidence level.

The optimal profit profiles, SCPP2 (single chance profit profile 2) and JCPP2 (joint chance profit profile 2), shown in Fig. 3 were measured at different confidence levels. In SCPP2, the single chance constraints,  $C_{5+}$  ( $k=5$ ),  $N_2$  ( $k=6$ ) and  $CO_2$  ( $k=7$ ), were all held at the 99% confidence level, whereas the remaining single chance constraints,  $C_1$  ( $k=1$ ),  $C_2$  ( $k=2$ ),  $C_3$  ( $k=3$ ) and  $C_{4s}$  ( $k=4$ ), were varied from the 50% to 100% confidence levels. Similarly, for JCPP2, the constraints,  $C_{5+}$ ,  $N_2$  and  $CO_2$ , were held at the 99% confidence level, whereas the remaining constraints were varied from the 50% to 100% confidence level.

The equations shown in (B-9)–(B-15) can be calculated by repeatedly varying the confidence level. On the other hand, to calculate the relaxed joint chance constrained shown in Eq. (B-16), the parameter ( $r_k^\xi$ ) in the probability distribution function first needs to be converted to the corresponding standard form by taking the mean and standard deviation of the uncertain parameter ( $\xi_k$ ). Once  $r_k^\xi$  is expressed in standard form, the next step is a calculation using a special function called 'errorf', which is found in GAMS (Rosenthal, 2006).

The optimal profit profiles in Fig. 3 decreased slowly until it reached the critical point,  $\alpha_c = 0.95$ . Therefore, moving further from this point,  $\alpha_c$ , to the right direction guarantees the reliability of the process but the profit decreases dramatically. On the

other hand, moving from  $\alpha_c$  to the left direction improves the profitability, but at the expense of the process reliability. This also supports the concept of the Pareto optimality, in which the actual choice of the optimal value depends on the relative reliability and expected profit. Therefore, according to the Pareto principle, the reliability of holding the process constraints is better only by reducing the profit to a certain level.

Consider the case in Fig. 3 where someone wishes to decide at the 50% confidence level using SCPP1, the corresponding profit value at this point is the highest among all other optimal points along the profit profile path. On the other hand, there is also a 50% probability for the violation constraints to occur, which is a deterministic optimization decision. Similarly, if someone wishes to decide at the 75% confidence level using SCPP1, there is still a 25% probability for any possible violations of the constraint to occur. Therefore, there should be a trade-off point that can be determined by holding both the reliability of the process and profitability of the plant. Based on this, the 95% confidence level will be a suitable choice that can compromise both the reliability of the process and profitability of the plant. With this decision, there is only a 5% risk of violation of the constraint.

Finding the critical or trade-off point is related to the data measurement. For SCPP1, all the single chance constraints were varied with the 5% confidence level interval (50%, 55%, ..., 100%). In such a case, there is a 'rule of thumb' to pre-determine the critical point, which is by subtracting the 5% confidence level interval from the 100% confidence level. For example, if the data in the above case was varied at the 10% confidence level interval, the trade-off point would have been at the 90% confidence level (100% – 10%). On the other hand, this might not be true when each single chance constraint is held at different confidence levels, which are generally difficult to plot even if it is easy to find the numerical value for the optimal solution.

The optimal profit profile, SCPP2 and JCPP2, has a lower profit value compared to SCPP1 and JCPP1, respectively. This is because more emphasis was given to holding some of the constraints ( $C_{5+}$ ,  $N_2$  and  $CO_2$ ) at the 99% confidence level. Such optimization is referred as the 'worst-case' optimization. The advantage of 'worst-case' optimization is that it is very good in holding the constraints with a minimal risk of violation. Nevertheless, there is also a drastic profit reduction at the expense of having a reliable process constraint (Li, Wendt, et al., 2004).

The optimal profit profile SCPP2 and JCPP2 have given a lower profit value compared to both SCPP1 and JCPP1, respectively. This is due to the fact that more emphasis was given to hold some of the constraints ( $C_{5+}$ ,  $N_2$  and  $CO_2$ ) at 99% confidence level. Such kind of optimization is referred as 'worst-case' optimization. The advantage of 'worst-case' optimization is that it is very good in holding the constraints with minimum risk of violation. However, there is also a drastic profit reduction at the expense of having a reliable process constraint (Li, Wendt, et al., 2004).

Consider the single chance constrained optimization profit profile, SCPP1 in Fig. 3, the optimal profit values for the 50% and 100% confidence level were \$21,138 per hour and \$2088 per hour, respectively. The corresponding profit for the joint chance constrained optimization JCPP1 were \$18,203 per hour and \$2088 per hour, respectively. Accordingly, the difference in profit for the single chance constrained optimization at the 50% and 100% confidence level was \$19,050 per hour (\$21,138 per hour – \$2088 per hour). Similarly, the difference in profit for the joint chance constrained optimization at the 50% and 100% confidence level gave \$16,115 per hour (\$18,203 per hour – \$2088 per hour). The difference in profit for the single chance constrained optimization (\$19,050 per hour) was higher than that of the joint chance-constrained optimization (\$16,115 per hour). Such profit differences arise due to the

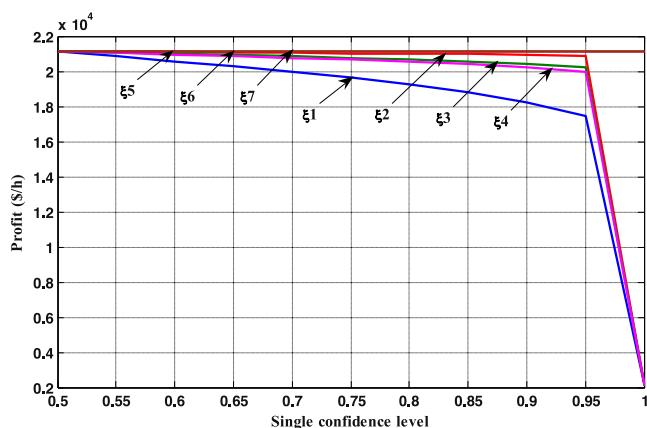


Fig. 4. Sensitivity analysis of profit for the uncertain feed case.

fact that the single chance constrained optimization has a more solution space than the joint chance-constrained optimization (Li et al., 2008).

Referring to Fig. 3, the optimal profit region for the single chance constrained optimization SCPP1 was in this interval: [\$21,138 per hour, \$2088 per hour]. For the joint chance constrained optimization JCPP1, the optimal profit value region was: [\$18,203 per hour, \$2088 per hour]. The corresponding optimal profit value, \$ 18,203 per hour, can be traced back in the single chance constrained optimization. This again shows that the solution space for the joint chance constrained optimization is a subset of the solution space for the single chance constrained optimization (Li et al., 2008).

### 5.1.3. Sensitivity analysis

Sensitivity analysis for profit was performed by taking each uncertain feed component flow ( $\xi_1, \xi_2, \dots, \xi_7$ ) as shown in Fig. 4. The analysis was made in such a way that one of the uncertain feed component flows was varied from the 50% to 100% confidence level, whereas all the remaining constraints were held at the 50% confidence level. For example, referring to Appendix B, consider the single chance constraints in Eqs. (B-7) and (B-15). Sensitivity analysis for the CO<sub>2</sub> component ( $k=7$ ) was performed by varying  $\xi_7$  from the 50% to 100% confidence level. In this case, the other constraints shown in Eqs. (B-9)–(B-14) were held at the 50% confidence level.

Sensitivity analysis for the other components can also be performed in similar manner. From Fig. 4, the optimal profit profile shows that the profit will not be affected if the optimal decision needs to be made at the 95% confidence level for the  $\xi_1, \xi_2, \xi_3$  and  $\xi_4$  cases. On the other hand, the optimal profit decision for  $\xi_5, \xi_6$  and  $\xi_7$  show that it is not affected at different single confidence levels. Such sensitivity analysis helps identify those uncertain feed component inflows that have significant impacts on the performance of the plant during plant operation. For example, the N<sub>2</sub> content in the feed affects the production of sales gas by reducing its BTU value. This is because the N<sub>2</sub> rich gases cannot be burned due to environmental constraints. Therefore, it is important to determine the optimal N<sub>2</sub> value in the feed so that its effect can be minimized from an environmental perspective. In addition, the CO<sub>2</sub> content of the feed has a significant effect on the performance of the plant unless it is optimized. The high CO<sub>2</sub> content in the feed might result in a risk of plugging in the demethanizer column. Furthermore, it will also affect the production of ethane in the demethanizer column.

### 5.2. Case study 2

The previous case study discussed the feeds involving uncertainty from the plant inlet. On the other hand, in the plant

Table 4

Mean and standard deviations of the uncertain product component outflow.

Components ( $k$ )	Uncertain feed component inflows ( $\zeta_k$ )	Mean (ton/h)	Standard deviation (ton/h)
C <sub>1</sub>	$\zeta_1$	–	–
C <sub>2</sub>	$\zeta_2$	0.291	0.153
C <sub>3</sub>	$\zeta_3$	24.486	5.027
C <sub>4s</sub>	$\zeta_4$	15.66	2.780
C <sub>5+</sub>	$\zeta_5$	0.156	0.136
N <sub>2</sub>	$\zeta_6$	–	–
CO <sub>2</sub>	$\zeta_7$	–	–

outlet, there are also some products, such as propane and butane, in which their product requirement or specifications can vary according to customer demand. These two products are mostly used as feed stock for petrochemical plants. The petrochemical plants can change the specifications of their feed stock owing to seasonal variations of the product demand or for some special order that the plant obtains from their customers. As a result, the composition of C<sub>2</sub>, C<sub>3</sub>, C<sub>4s</sub> and C<sub>5+</sub> in the products should meet the requirements to satisfy customer demand.

On the other hand, when the demand for propane is high and that of butane is depressed, the plant may need to shift its production mode and produce more propane. This ensures the plant continues to generate high revenue under particular demand conditions. Similarly, if the demand for LPG is high, both propane and butane will be needed to take advantage of the favorable market condition. Moreover, it is also advantageous to use the depropanizer column as a LPG column so that the debutanizer column can be shut down for energy saving purposes.

The PRU section for this case study is configured in such a way that the debutanizer column has been left out and the depropanizer column will operate as a LPG column. The deethanizer column set up is similar to the previous case study. Four feeds ( $R_1, R_2, R_3$  and  $R_4$ ) enter the plant in Fig. 2, where all the feeds are assumed to be decision variables. The products from the plant outlet for this case study are:  $P_1$  (sales gas),  $P_2$  (ethane),  $\hat{P}_{3,4}$  (LPG),  $P_5$  (condensate) and  $P_6$  (carbon dioxide).

### 5.2.1. Data analysis

Similar to case study 1, a large set of data with 8785 data points on an hourly basis for the uncertain LPG product  $\hat{P}_{3,4}$  has been taken. The seven feed components ( $k=1, \dots, 7$ ) in the LPG product ( $\hat{P}_{3,4}$ ) include C<sub>1</sub>, C<sub>2</sub>, C<sub>3</sub>, C<sub>4s</sub>, C<sub>5+</sub>, N<sub>2</sub> and CO<sub>2</sub>, respectively. Based on this, the normal distribution for the uncertain product component outflows has been assumed. Table 4 lists the mean and standard deviations of all the product component outflows. Table 5 shows the maximum values for the raw material and product flow, which are considered to be decision variables. The minimum values for those decision variables were set to zero. The expected price factor

Table 5

Maximum and minimum values of decision variables for uncertain product flow case.

Raw material and products	Maximum value (ton/h)
$R_1$	334.582
$R_2$	220.314
$R_3$	10.706
$R_4$	35.586
$P_1$	298.518
$P_2$	37.311
$P_5$	43.111
$P_6$	57.659

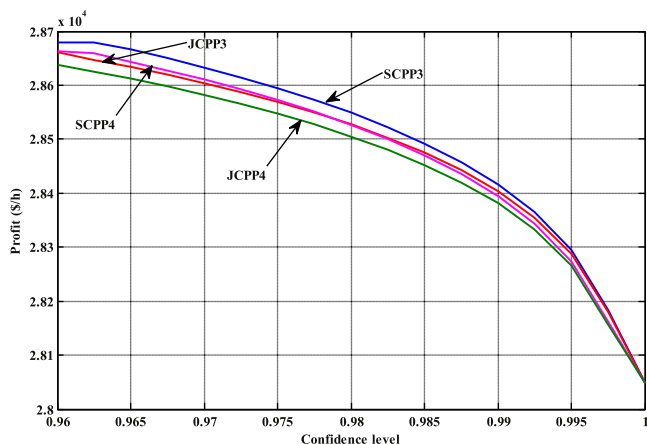


Fig. 5. Optimal profit profile for the uncertain product case.

in Table 3 remains the same except for the LPG product  $\hat{P}_{3,4}$  which is \$189.362 per ton.

### 5.2.2. Optimization

The optimization problems were formulated based on Eqs. (19)–(26). Both the single and joint chance optimization problems are presented in Appendix B (Eqs. (B-17)–(B-32)). Fig. 5 shows the optimal profit profiles starting from the 96% to 100% confidence level for the single and joint chance constrained optimization cases. The reason for plotting in such a confidence interval [0.96, 1] is that the profit shows a significant change within this range. As shown in Fig. 5, the data was varied with the 0.25% confidence level interval. Using the 'rule of thumb' discussed in case study 1, the critical or trade-off point can be pre-determined by subtracting from the 100% confidence level ( $100\% - 0.25\% = 99.75\%$ ). Thus, at the 99.75% confidence level, the profit begins to decrease drastically as shown in Fig. 5. The risk of a violation of the constraint by taking this decision was only 0.25%.

For the optimal profit profile, SCPP3 and JCCP3, the constraints were measured at the same confidence level. On the other hand, for the optimal profit profiles, SCPP4 and JCCP4, the  $C_2$  component and  $C_{5+}$  component were held at the 99% confidence level because these are impurities in the LPG product. The remaining constraints,  $C_3$  and  $C_{4s}$ , were varied from the 96% to 100% confidence level. Similar to the result obtained from the Case study 1, the optimal profit profile, SCPP4 and JCCP4, gives a lower profit value than SCPP3 and JCCP3, respectively. This is because the decision using SCPP4 and JCCP4 is the 'worst-case' scenario.

Consider the optimal single chance constrained profit profile SCPP1 shown in Fig. 3, the profit values at the 96% and 100% confidence level were \$14,706 per hour and \$2088 per hour, respectively. Accordingly, the profit was changed by 86% when moving from the 96% to 100% confidence level. By taking the same data at the 96% and 100% confidence level for the optimal single chance constrained profit profile SCPP3 shown in Fig. 5, the corresponding profit was \$28,662 per hour and \$28,047 per hour, respectively. In this case, the profit has been changed only by 2% as moving from the 96% to 100% confidence levels. This also shows that the change in profit for uncertainty from the plant inlet is much higher than that of the plant outlet (Li et al., 2008).

### 5.2.3. Sensitivity analysis

Fig. 6 presents the results of sensitivity analysis for profit by varying the single confidence level. Such sensitivity analysis is made by varying each individual constraint separately from the 96% to 100% confidence level. Sensitivity analysis for  $\zeta_3$  was made

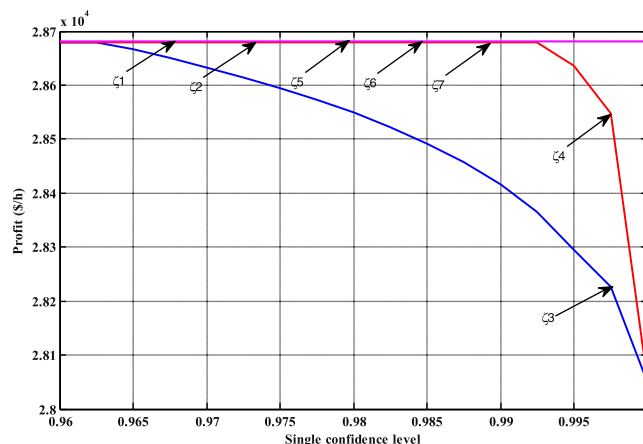


Fig. 6. Sensitivity analysis of profit for the uncertain product case.

by treating the constraint in Eq. (B-27), as shown in Appendix B, and allowing the confidence level to vary from 96% to 100%. The remaining constraints were held at the 96% confidence level. The same analysis was performed for  $\zeta_4$  by varying the constraint in Eq. (B-28) from the 96% to 100% confidence level.

The profit profile for  $\zeta_3$  and  $\zeta_4$  show that how these two uncertain variables can affect the profit. The sensitivity result from the remaining product components ( $\zeta_1$ ,  $\zeta_2$ ,  $\zeta_5$ ,  $\zeta_6$  and  $\zeta_7$ ) shows that the profit remains constant because the value of these components is normally small and their content in the LPG product is almost negligible.

## 6. Conclusions

Uncertainty is an inherent characteristic of any chemical process plant that profoundly affects the economics of the plant. Such an uncertainty effect can be incorporated using chance constrained models. By using chance constrained optimization, the optimum trade-off for the reliability of holding the process constraints and profitability of the plant can be determined by repeatedly solving the optimization problem. The reliability of holding the process constraints can be now measured with the "unit" called the confidence or probability level. Two case studies were considered for an existing gas processing plant. Based on the results obtained from the two case studies, the uncertainty from the plant inlet has a significant impact on the overall economic performance of the plant compared to the plant outlet case. Accordingly, the profit was changed by 86% for the inlet uncertainty case. On the other hand, the profit change for the outlet uncertainty case was only 2% for the same confidence level interval taken. The sensitivity study from both case studies helps to identify those key components which have a greater or lesser impact on the overall plant profit. In addition, it also assists in solving the problems related to plant operation by optimizing the quantity of unwanted components that enter the plant.

## Acknowledgments

The authors wish to thank Universiti Teknologi PETRONAS for the research grant used for this project. The authors are also grateful to Yeungnam University and Curtin University Sarawak Malaysia for the materials used during the preparation of this study.

## Appendix A. Historical plant data

See Figs. A1–A3.



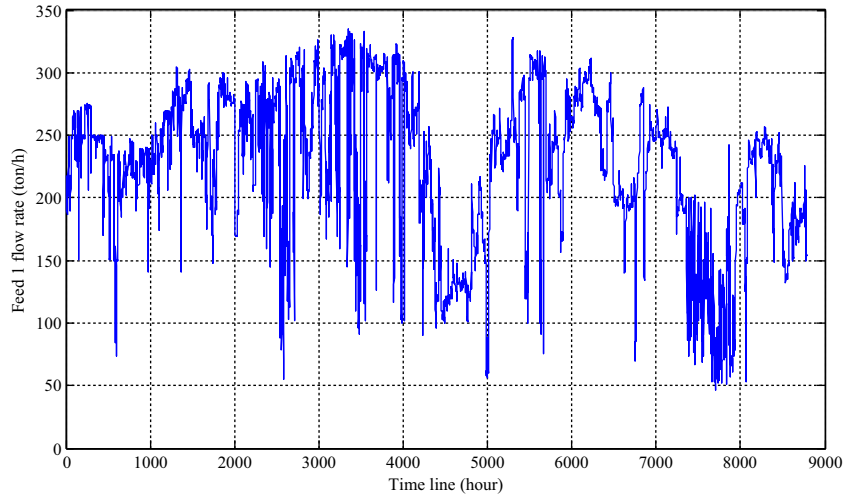


Fig. A1. Feed 1 ( $\hat{R}_1$ ) plant history data in a yearly basis.

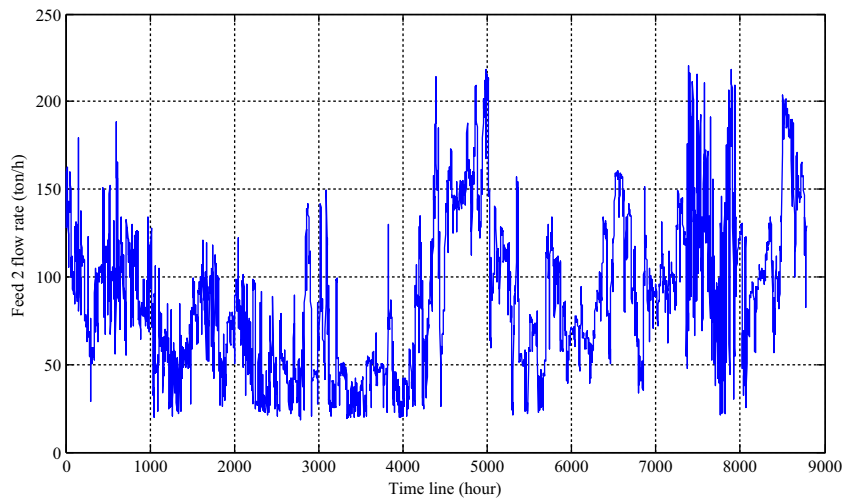


Fig. A2. Feed 2 ( $\hat{R}_2$ ) plant history data in a yearly basis.

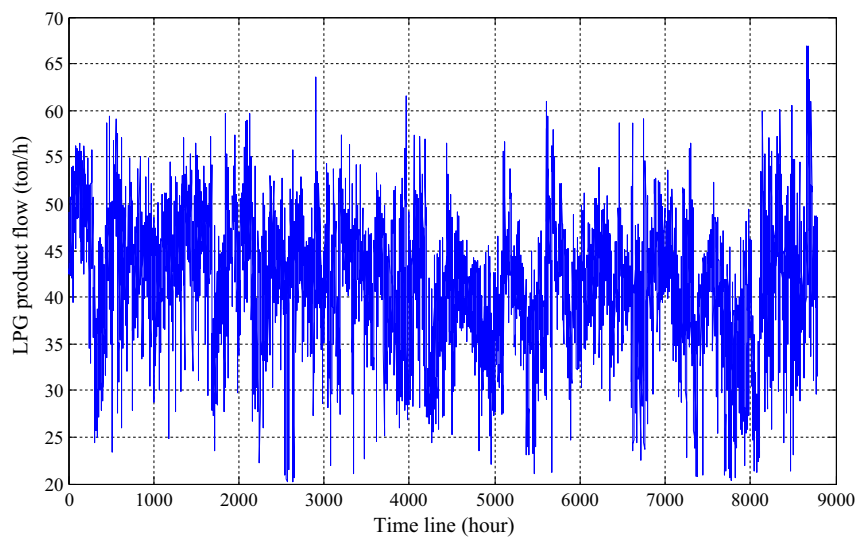


Fig. A3. LPG product ( $\hat{P}_{3,4}$ ) plant history data in a yearly basis.

**Appendix B. Optimization problem formulation for the case studies**

**B.1. Case study 1**

The optimization problem formulation for this case study begins by looking to Eqs. (10)–(17). Based on Eq. (12), the single chance constraints can be expressed as:

For  $k = 1$ :  $C_1$  component:

$$Pr_1\{r_1^{\xi} = a_{1,1}P_1 + a_{1,2}P_2 + a_{1,3}P_3 + a_{1,4}P_4 + a_{1,5}P_5 + a_{1,6}P_6 - b_{1,3}R_3 - b_{1,3}R_4 \leq \xi_1\} \geq \alpha_1 \tag{B-1}$$

For  $k = 2$ :  $C_2$  component:

$$Pr_2\{r_2^{\xi} = a_{2,1}P_1 + a_{2,2}P_2 + a_{2,3}P_3 + a_{2,4}P_4 + a_{2,5}P_5 + a_{2,6}P_6 - b_{2,3}R_3 - b_{2,3}R_4 \leq \xi_2\} \geq \alpha_2 \tag{B-2}$$

For  $k = 3$ :  $C_3$  component:

$$Pr_3\{r_3^{\xi} = a_{3,1}P_1 + a_{3,2}P_2 + a_{3,3}P_3 + a_{3,4}P_4 + a_{3,5}P_5 + a_{3,6}P_6 - b_{3,3}R_3 - b_{3,3}R_4 \leq \xi_3\} \geq \alpha_3 \tag{B-3}$$

For  $k = 4$ :  $C_{45}$  component:

$$Pr_4\{r_4^{\xi} = a_{4,1}P_1 + a_{4,2}P_2 + a_{4,3}P_3 + a_{4,4}P_4 + a_{4,5}P_5 + a_{4,6}P_6 - b_{4,3}R_3 - b_{4,3}R_4 \leq \xi_4\} \geq \alpha_4 \tag{B-4}$$

For  $k = 5$ :  $C_{5+}$  component:

$$Pr_5\{r_5^{\xi} = a_{5,1}P_1 + a_{5,2}P_2 + a_{5,3}P_3 + a_{5,4}P_4 + a_{5,5}P_5 + a_{5,6}P_6 - b_{5,3}R_3 - b_{5,3}R_4 \leq \xi_5\} \geq \alpha_5 \tag{B-5}$$

For  $k = 6$ :  $N_2$  component:

$$Pr_6\{r_6^{\xi} = a_{6,1}P_1 + a_{6,2}P_2 + a_{6,3}P_3 + a_{6,4}P_4 + a_{6,5}P_5 + a_{6,6}P_6 - b_{6,3}R_3 - b_{6,3}R_4 \leq \xi_6\} \geq \alpha_6 \tag{B-6}$$

For  $k = 7$ :  $CO_2$  component:

$$Pr_7\{r_7^{\xi} = a_{7,1}P_1 + a_{7,2}P_2 + a_{7,3}P_3 + a_{7,4}P_4 + a_{7,5}P_5 + a_{7,6}P_6 - b_{7,3}R_3 - b_{7,3}R_4 \leq \xi_7\} \geq \alpha_7 \tag{B-7}$$

Similarly, based on Eq. (13), the joint chance constraints become:

$$Pr \left\{ \begin{array}{l} r_1^{\xi} = a_{1,1}P_1 + a_{1,2}P_2 + a_{1,3}P_3 + a_{1,4}P_4 + a_{1,5}P_5 + a_{1,6}P_6 - b_{1,3}R_3 - b_{1,3}R_4 \leq \xi_1 \\ r_2^{\xi} = a_{2,1}P_1 + a_{2,2}P_2 + a_{2,3}P_3 + a_{2,4}P_4 + a_{2,5}P_5 + a_{2,6}P_6 - b_{2,3}R_3 - b_{2,3}R_4 \leq \xi_2 \\ r_3^{\xi} = a_{3,1}P_1 + a_{3,2}P_2 + a_{3,3}P_3 + a_{3,4}P_4 + a_{3,5}P_5 + a_{3,6}P_6 - b_{3,3}R_3 - b_{3,3}R_4 \leq \xi_3 \\ r_4^{\xi} = a_{4,1}P_1 + a_{4,2}P_2 + a_{4,3}P_3 + a_{4,4}P_4 + a_{4,5}P_5 + a_{4,6}P_6 - b_{4,3}R_3 - b_{4,3}R_4 \leq \xi_4 \\ r_5^{\xi} = a_{5,1}P_1 + a_{5,2}P_2 + a_{5,3}P_3 + a_{5,4}P_4 + a_{5,5}P_5 + a_{5,6}P_6 - b_{5,3}R_3 - b_{5,3}R_4 \leq \xi_5 \\ r_6^{\xi} = a_{6,1}P_1 + a_{6,2}P_2 + a_{6,3}P_3 + a_{6,4}P_4 + a_{6,5}P_5 + a_{6,6}P_6 - b_{6,3}R_3 - b_{6,3}R_4 \leq \xi_6 \\ r_7^{\xi} = a_{7,1}P_1 + a_{7,2}P_2 + a_{7,3}P_3 + a_{7,4}P_4 + a_{7,5}P_5 + a_{7,6}P_6 - b_{7,3}R_3 - b_{7,3}R_4 \leq \xi_7 \end{array} \right\} \geq \alpha \tag{B-8}$$

The relaxed or equivalent deterministic form based on Eq. (16) for the single chance constraints shown in Eqs. (B-1)–(B-7) becomes:

$$a_{1,1}P_1 + a_{1,2}P_2 + a_{1,3}P_3 + a_{1,4}P_4 + a_{1,5}P_5 + a_{1,6}P_6 - b_{1,3}R_3 - b_{1,3}R_4 \leq \Phi^{-1}(1 - \alpha_1) \tag{B-9}$$

$$a_{2,1}P_1 + a_{2,2}P_2 + a_{2,3}P_3 + a_{2,4}P_4 + a_{2,5}P_5 + a_{2,6}P_6 - b_{2,3}R_3 - b_{2,3}R_4 \leq \Phi^{-1}(1 - \alpha_2) \tag{B-10}$$

$$a_{3,1}P_1 + a_{3,2}P_2 + a_{3,3}P_3 + a_{3,4}P_4 + a_{3,5}P_5 + a_{3,6}P_6 - b_{3,3}R_3 - b_{3,3}R_4 \leq \Phi^{-1}(1 - \alpha_3) \tag{B-11}$$

$$a_{4,1}P_1 + a_{4,2}P_2 + a_{4,3}P_3 + a_{4,4}P_4 + a_{4,5}P_5 + a_{4,6}P_6 - b_{4,3}R_3 - b_{4,3}R_4 \leq \Phi^{-1}(1 - \alpha_4) \tag{B-12}$$

$$a_{5,1}P_1 + a_{5,2}P_2 + a_{5,3}P_3 + a_{5,4}P_4 + a_{5,5}P_5 + a_{5,6}P_6 - b_{5,3}R_3 - b_{5,3}R_4 \leq \Phi^{-1}(1 - \alpha_5) \tag{B-13}$$

$$a_{6,1}P_1 + a_{6,2}P_2 + a_{6,3}P_3 + a_{6,4}P_4 + a_{6,5}P_5 + a_{6,6}P_6 - b_{6,3}R_3 - b_{6,3}R_4 \leq \Phi^{-1}(1 - \alpha_6) \tag{B-14}$$

$$a_{7,1}P_1 + a_{7,2}P_2 + a_{7,3}P_3 + a_{7,4}P_4 + a_{7,5}P_5 + a_{7,6}P_6 - b_{7,3}R_3 - b_{7,3}R_4 \leq \Phi^{-1}(1 - \alpha_7) \tag{B-15}$$

The relaxation for the joint chance constraints in Eq. (B-8) based on Eq. (17) gives:

$$\left[ \begin{array}{l} (1 - \Phi(a_{1,1}P_1 + a_{1,2}P_2 + a_{1,3}P_3 + a_{1,4}P_4 + a_{1,5}P_5 + a_{1,6}P_6 - b_{1,3}R_3 - b_{1,3}R_4)) \\ (1 - \Phi(a_{2,1}P_1 + a_{2,2}P_2 + a_{2,3}P_3 + a_{2,4}P_4 + a_{2,5}P_5 + a_{2,6}P_6 - b_{2,3}R_3 - b_{2,3}R_4)) \\ (1 - \Phi(a_{3,1}P_1 + a_{3,2}P_2 + a_{3,3}P_3 + a_{3,4}P_4 + a_{3,5}P_5 + a_{3,6}P_6 - b_{3,3}R_3 - b_{3,3}R_4)) \\ (1 - \Phi(a_{4,1}P_1 + a_{4,2}P_2 + a_{4,3}P_3 + a_{4,4}P_4 + a_{4,5}P_5 + a_{4,6}P_6 - b_{4,3}R_3 - b_{4,3}R_4)) \\ (1 - \Phi(a_{5,1}P_1 + a_{5,2}P_2 + a_{5,3}P_3 + a_{5,4}P_4 + a_{5,5}P_5 + a_{5,6}P_6 - b_{5,3}R_3 - b_{5,3}R_4)) \\ (1 - \Phi(a_{6,1}P_1 + a_{6,2}P_2 + a_{6,3}P_3 + a_{6,4}P_4 + a_{6,5}P_5 + a_{6,6}P_6 - b_{6,3}R_3 - b_{6,3}R_4)) \\ (1 - \Phi(a_{7,1}P_1 + a_{7,2}P_2 + a_{7,3}P_3 + a_{7,4}P_4 + a_{7,5}P_5 + a_{7,6}P_6 - b_{7,3}R_3 - b_{7,3}R_4)) \end{array} \right] \geq \alpha \quad (\text{B-16})$$

### B.2. Case study 2

The optimization problem formulation for case study 2 is based on Eqs. (19)–(26). The single chance constraints formulation based on Eq. (21) gives:

For  $k=1$ :  $C_1$  component:

$$Pr_1\{p_1^\zeta = b_{1,1}R_1 + b_{1,2}R_2 + b_{1,3}R_3 + b_{1,4}R_4 - a_{1,1}P_1 - a_{1,2}P_2 - a_{1,5}P_5 - a_{1,6}P_6 \geq \zeta_1\} \geq \alpha_1 \quad (\text{B-17})$$

For  $k=2$ :  $C_2$  component:

$$Pr_2\{p_2^\zeta = b_{2,1}R_1 + b_{2,2}R_2 + b_{2,3}R_3 + b_{2,4}R_4 - a_{2,1}P_1 - a_{2,2}P_2 - a_{2,5}P_5 - a_{2,6}P_6 \geq \zeta_2\} \geq \alpha_2 \quad (\text{B-18})$$

For  $k=3$ :  $C_3$  component:

$$Pr_3\{p_3^\zeta = b_{3,1}R_1 + b_{3,2}R_2 + b_{3,3}R_3 + b_{3,4}R_4 - a_{3,1}P_1 - a_{3,2}P_2 - a_{3,5}P_5 - a_{3,6}P_6 \geq \zeta_3\} \geq \alpha_3 \quad (\text{B-19})$$

For  $k=4$ :  $C_{4s}$  component:

$$Pr_4\{p_4^\zeta = b_{4,1}R_1 + b_{4,2}R_2 + b_{4,3}R_3 + b_{4,4}R_4 - a_{4,1}P_1 - a_{4,2}P_2 - a_{4,5}P_5 - a_{4,6}P_6 \geq \zeta_4\} \geq \alpha_4 \quad (\text{B-20})$$

For  $k=5$ :  $C_{5+}$  component:

$$Pr_5\{p_5^\zeta = b_{5,1}R_1 + b_{5,2}R_2 + b_{5,3}R_3 + b_{5,3}R_4 - a_{5,1}P_1 - a_{5,2}P_2 - a_{5,5}P_5 - a_{5,6}P_6 \geq \zeta_5\} \geq \alpha_5 \quad (\text{B-21})$$

For  $k=6$ :  $N_2$  component:

$$Pr_6\{p_6^\zeta = b_{6,1}R_1 + b_{6,2}R_2 + b_{6,3}R_3 + b_{6,3}R_4 - a_{6,1}P_1 - a_{6,2}P_2 - a_{6,5}P_5 - a_{6,6}P_6 \geq \zeta_6\} \geq \alpha_6 \quad (\text{B-22})$$

For  $k=7$ :  $CO_2$  component:

$$Pr_7\{p_7^\xi = b_{7,1}R_1 + b_{7,2}R_2 + b_{7,3}R_3 + b_{7,3}R_4 - a_{7,1}P_1 - a_{7,2}P_2 - a_{7,5}P_5 - a_{7,6}P_6 \geq \zeta_7\} \geq \alpha_7 \quad (\text{B-23})$$

The joint chance constraints formulation based on Eq. (22) becomes:

$$Pr \left\{ \begin{array}{l} p_1^\zeta = b_{1,1}R_1 + b_{1,2}R_2 + b_{1,3}R_3 + b_{1,4}R_4 - a_{1,1}P_1 - a_{1,2}P_2 - a_{1,5}P_5 - a_{1,6}P_6 \geq \zeta_1 \\ p_2^\zeta = b_{2,1}R_1 + b_{2,2}R_2 + b_{2,3}R_3 + b_{2,4}R_4 - a_{2,1}P_1 - a_{2,2}P_2 - a_{2,5}P_5 - a_{2,6}P_6 \geq \zeta_2 \\ p_3^\zeta = b_{3,1}R_1 + b_{3,2}R_2 + b_{3,3}R_3 + b_{3,4}R_4 - a_{3,1}P_1 - a_{3,2}P_2 - a_{3,5}P_5 - a_{3,6}P_6 \geq \zeta_3 \\ p_4^\zeta = b_{4,1}R_1 + b_{4,2}R_2 + b_{4,3}R_3 + b_{4,4}R_4 - a_{4,1}P_1 - a_{4,2}P_2 - a_{4,5}P_5 - a_{4,6}P_6 \geq \zeta_4 \\ p_5^\zeta = b_{5,1}R_1 + b_{5,2}R_2 + b_{5,3}R_3 + b_{5,3}R_4 - a_{5,1}P_1 - a_{5,2}P_2 - a_{5,5}P_5 - a_{5,6}P_6 \geq \zeta_5 \\ p_6^\zeta = b_{6,1}R_1 + b_{6,2}R_2 + b_{6,3}R_3 + b_{6,3}R_4 - a_{6,1}P_1 - a_{6,2}P_2 - a_{6,5}P_5 - a_{6,6}P_6 \geq \zeta_6 \\ p_7^\xi = b_{7,1}R_1 + b_{7,2}R_2 + b_{7,3}R_3 + b_{7,3}R_4 - a_{7,1}P_1 - a_{7,2}P_2 - a_{7,5}P_5 - a_{7,6}P_6 \geq \zeta_7 \end{array} \right\} \geq \alpha \quad (\text{B-24})$$

The corresponding relaxation based on Eq. (25) for the single chance constrained shown in Eqs. (B-17)–(B-23) becomes:

$$b_{1,1}R_1 + b_{1,2}R_2 + b_{1,3}R_3 + b_{1,4}R_4 - a_{1,1}P_1 - a_{1,2}P_2 - a_{1,5}P_5 - a_{1,6}P_6 \geq \Phi^{-1}(\alpha_1) \quad (\text{B-25})$$

$$b_{2,1}R_1 + b_{2,2}R_2 + b_{2,3}R_3 + b_{2,4}R_4 - a_{2,1}P_1 - a_{2,2}P_2 - a_{2,5}P_5 - a_{2,6}P_6 \geq \Phi^{-1}(\alpha_2) \quad (\text{B-26})$$

$$b_{3,1}R_1 + b_{3,2}R_2 + b_{3,3}R_3 + b_{3,4}R_4 - a_{3,1}P_1 - a_{3,2}P_2 - a_{3,5}P_5 + a_{3,6}P_6 \geq \Phi^{-1}(\alpha_3) \quad (\text{B-27})$$

$$b_{4,1}R_1 + b_{4,2}R_2 + b_{4,3}R_3 + b_{4,4}R_4 - a_{4,1}P_1 - a_{4,2}P_2 - a_{4,5}P_5 - a_{4,6}P_6 \geq \Phi^{-1}(\alpha_4) \quad (\text{B-28})$$

$$b_{5,1}R_1 + b_{5,2}R_2 + b_{5,3}R_3 + b_{5,3}R_4 - a_{5,1}P_1 - a_{5,2}P_2 - a_{5,5}P_5 - a_{5,6}P_6 \geq \Phi^{-1}(\alpha_5) \quad (\text{B-29})$$

$$b_{6,1}R_1 + b_{6,2}R_2 + b_{6,3}R_3 + b_{6,3}R_4 - a_{6,1}P_1 - a_{6,2}P_2 - a_{6,5}P_5 - a_{6,6}P_6 \geq \Phi^{-1}(\alpha_6) \quad (\text{B-30})$$

$$b_{7,1}R_1 + b_{7,2}R_2 + b_{7,3}R_3 + b_{7,3}R_4 - a_{7,1}P_1 - a_{7,2}P_2 - a_{7,5}P_5 - a_{7,6}P_6 \geq \Phi^{-1}(\alpha_7) \quad (\text{B-31})$$

The relaxation based on Eq. (26) for the joint chance constraints shown in Eq. (B-24) becomes:

$$\begin{bmatrix} (\Phi(b_{1,1}R_1 + b_{1,2}R_2 + b_{1,3}R_3 + b_{1,4}R_4 - a_{1,1}P_1 - a_{1,2}P_2 - a_{1,5}P_5 - a_{1,6}P_6)) \\ (\Phi(b_{2,1}R_1 + b_{2,2}R_2 + b_{2,3}R_3 + b_{2,4}R_4 - a_{2,1}P_1 - a_{2,2}P_2 - a_{2,5}P_5 - a_{2,6}P_6)) \\ (\Phi(b_{3,1}R_1 + b_{3,2}R_2 + b_{3,3}R_3 + b_{3,4}R_4 - a_{3,1}P_1 - a_{3,2}P_2 - a_{3,5}P_5 - a_{3,6}P_6)) \\ (\Phi(b_{4,1}R_1 + b_{4,2}R_2 + b_{4,3}R_3 + b_{4,4}R_4 - a_{4,1}P_1 - a_{4,2}P_2 - a_{4,5}P_5 - a_{4,6}P_6)) \\ (\Phi(b_{6,1}R_1 + b_{6,2}R_2 + b_{6,3}R_3 + b_{6,3}R_4 - a_{6,1}P_1 - a_{6,2}P_2 - a_{6,5}P_5 - a_{6,6}P_6)) \\ (\Phi(b_{5,1}R_1 + b_{5,2}R_2 + b_{5,3}R_3 + b_{5,3}R_4 - a_{5,1}P_1 - a_{5,2}P_2 - a_{5,5}P_5 - a_{5,6}P_6)) \\ (\Phi(b_{7,1}R_1 + b_{7,2}R_2 + b_{7,3}R_3 + b_{7,3}R_4 - a_{7,1}P_1 - a_{7,2}P_2 - a_{7,5}P_5 - a_{7,6}P_6)) \end{bmatrix} \geq \alpha \quad (\text{B-32})$$

## References

- Ahmed, S., & Sahinidis, N. V. (1998). Robust process planning under uncertainty? *Industrial & Engineering Chemistry Research*, 37(5), 1883–1892.
- Arellano-Garcia, H., Wendt, M., Li, P., & Wozny, G. (2003). An evaluation strategy for optimal operation of batch processes under uncertainties by probabilistic programming. In B. Chen, & A. W. Westerberg (Eds.), *PSE8 proceedings* (pp. 148–153). Kunming: Elsevier.
- Arellano-Garcia, H., & Wozny, G. (2009). Chance constrained optimization of process systems under uncertainty: I. Strict monotonicity. *Computers & Chemical Engineering*, 33(10), 1568–1583.
- ASPEN HYSYS. (2006). *A user guide manual*. Burlington, MA: Aspen Technology.
- Diwaker, U. M. (2008). *Introduction to applied optimization*. New York: Springer-Verlag.
- Grossmann, I. E., Halemane, K. P., & Swaney, R. E. (1983). Optimization strategies for flexible chemical processes. *Computers & Chemical Engineering*, 7(3), 439–462.
- Gupta, A., & Maranas, C. D. (2000). A two-stage modeling and solution framework for multitude midterm planning under demand uncertainty. *Industrial & Engineering Chemistry Research*, 39(10), 3799–3813.
- Ierapetritou, M. G., Acevedo, J., & Pistikopoulos, E. N. (1996). An optimization approach for process engineering problems under uncertainty. *Computers & Chemical Engineering*, 20, 703–709.
- Li, P., Arellano-Garcia, H., & Wozny, G. (2008). Chance constrained programming approach to process optimization under uncertainty. *Computers & Chemical Engineering*, 32, 25–45.
- Li, W., Hui, C. W., Li, P., & Li, A. X. (2004). Refinery planning under uncertainty. *Industrial Engineering & Chemical Research*, 43, 6742–6755.
- Li, P., Wendt, M., & Wozny, G. (2004). Optimal planning for chemical engineering processes under uncertain market conditions. *Chemical Engineering & Technology*, 27, 641–651.
- Li, Z., & Ierapetritou, M. (2008). Process scheduling under uncertainty: Review and challenges. *Computers & Chemical Engineering*, 32(4–5), 715–727.
- Liu, M. L., & Sahinidis, N. V. (1996). Optimization in process planning under uncertainty. *Industrial Engineering & Chemical Research*, 43, 6742–6755.
- Mesfin, G., & Shuhaimi, M. (2010). A chance constrained approach for a gas processing plant with uncertain feed conditions. *Computers & Chemical Engineering*, 34(8), 1256–1267.
- Mesfin, G., Shuhaimi, M., & Lee, M. (2012). Analyzing the effects of uncertainties on the economic performance of a chemical process plant using a probabilistic optimization technique. *Computer Aided Chemical Engineering*, 30, 832–836.
- Petkov, S. B., & Maranas, C. (1997). Multiperiod planning and scheduling of multiproduct batch plants under demand uncertainty. *Industrial Engineering & Chemical Research*, 36, 4864–4881.
- Sahinidis, N. V. (2004). Optimization under uncertainty: State-of-the-art and opportunities. *Computers & Chemical Engineering*, 28, 971–983.
- Swaney, R. E., & Grossmann, I. E. (1985a). An index for operational flexibility in chemical process design. Part I: Formulation and theory. *AIChE Journal*, 31(4), 621–630.
- Swaney, R. E., & Grossmann, I. E. (1985b). An index for operational flexibility in chemical process design. Part II: Computational algorithms. *AIChE Journal*, 31(4), 631–641.
- Rosenthal, R. E. (2006). *A user's guide (tutorial)*. Washington, DC, USA: GAMS Development Corporation.
- Wendt, M., Li, P., & Wozny, G. (2002). Nonlinear chance constrained process optimization under uncertainty. *Industrial Engineering & Chemical Research*, 41, 3621–3629.