DESIGN OF PLASTICS SEPARATION SYSTEMS UNDER UNCERTAINTY BY THE SAMPLE AVERAGE APPROXIMATION METHOD

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ABSTRACT

This paper is an application of the systematic design approach to the plastics separation systems synthesis under uncertainty. The problem is distinguished from the traditional chemical distillation processes in that, first there are many separation mechanisms can be used and a combination of them is a necessity and second there is a significant variation of feed composition leading to the design of a flexible system crucial. The problem is formulated as a stochastic MINLP, which is solved by the sample average approximation method proposed previously by the authors. The method can handle large uncertainty space and determine appropriate sample sizes needed, therefore making the systems design under uncertainty of realistic size possible.

INTRODUCTION

Plastics recycling will play an increasingly important role in the design of effective product recovery systems. The synthesis of a plastics separation flowsheet is similar to the traditional distillation problems in terms of the need to determine the optimal separation sequence and unit parameters. The former is still challenging mainly due to the following two issues. First, a plastic mix can be separated by different mechanisms (for example, by the difference of density or polarity or surface tension). Therefore there are several types of equipment to choose from. Moreover, particles in a batch are not identical due to both the variation of particle properties (size, density, charge etc.) and the random performance in the separation units, such as the diffusion in the settling process, contacts with bubbles in the froth flotation units and entering position in the electrostatic separators. Second, there are many sources of uncertainties, such as feed composition, prices etc. In particular, the large variation of the feed composition, which can have a significant impact on the process feasibility and product quality, is intrinsic in this problem because the feed is usually a mix of various products in varying fractions.

For the first issue, a modeling approach has been developed in Wei and Realff (2003a-c) for many separation mechanisms, which takes account of the distribution of particle properties and other random factors. The approach embedded the influences of distribution parameters into separation models which have a unified form.

To approach the second challenge systematically, the problem is formulated as a stochastic mixed integer nonlinear program (sMINLP).

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$$
\begin{aligned}
v^* = \min_{x,y,z_i}\ & E_\theta\left[f\left(x, y, z_i, \theta_i\right)\right] \\
s.t.\ \ & g_j\left(x, y, z_{i,} \theta_i\right) \le 0 \quad \forall j \in J \\
& x \in X,\ z \in Z, y \in \{0,1\}^m \\
& \theta \in \Theta
\end{aligned}
\qquad \text{(SMINLP)}
$$

Where y is a vector of binary 0-1 variables denoting the choice of the units or the existence of the streams, x is a vector of design variables such as unit sizes, z is a vector of control/state variables, which can vary over periods/scenarios, and θ represents a vector of uncertain parameters. The constraint set J includes mass balances, unit design/operating models, design/operating specifications and some logical constraints. The expected value is often approximated through sample average by Monte Carlo method (Shapiro et al 2000), which transforms the stochastic problem into a deterministic one.

$$
\begin{aligned}
\hat{v}_N = \min_{x,z_i} & \frac{1}{N}\sum_{i=1}^{N}\left[f\left(x, y, z_i, \theta_i\right)\right] \\
s.t.\ \ & g_j\left(x, y, z_{i,} \theta_i\right) \le 0 \quad \forall i \in I_k; \forall j \in J \\
& x \in X,\ z \in Z
\end{aligned}
\qquad \text{(SAA-MINLP)}
$$

The above SAA-MINLP is solved by the Sample Average Approximation method (SAA) proposed by Wei and Realff (2004). A major problem in previous solution techniques is the lack of a method to determine the confidence of the solution, and the inability to consider a large number of uncertain parameters due to the computational complexity of the problem. Therefore, the sample size was usually chosen to be sufficiently large subject to the problem can still be solved in a reasonable time frame. The sample size could be under or over estimated, resulting in a poor solution quality or unnecessarily long computational time. The SAA method determines the sample size based on the confidence interval of the optimality gaps, constructed from solutions of replicates of smaller sample size problems and a larger sample size problem. The values of the decision variables are found from the smaller sample size problems and are fixed in the larger sample size problems, therefore, the scenarios of the larger sample size problems are decoupled, which contributes to significant computational savings. In the next section, we briefly introduce this algorithm and discuss some computational issues. Then the following section presents its application to the plastics separation problem. The last section concludes the paper.

THE ALGORITHM

Sample average approximation method for stochastic convex MINLPs

The basic idea of the sample average approximation method is to construct confidence intervals of the stochastic bounds.

The upper bound of a stochastic program can be found relatively easily since any feasible solution is an upper bound. The confidence interval for the upper bound is simply

$$v_{N'} \pm t_{N'-1,\alpha/2}\frac{S_{N'}}{\sqrt{N'}}$$

where, $v_{N'}$ is the objective value of a N'-sample size problem at any feasible solution,

$$v_{N'} = \frac{1}{N'}\sum_{i=1}^{N'} f_i \text{ , and } \frac{S_{N'}}{\sqrt{N'}} = \frac{1}{\sqrt{N'(N'-1)}}\sqrt{\sum_{i=1}^{N'}\left(f_i - v_{N'}\right)^2}$$

A widely used lower bounding technique (Mak et al., 1999; Kleywegt et al 2001; Norkin et al 1998) is to take advantage of the following fact:

$$E\left[\min_{x\in X} f(x)\right] \le \min_{x\in X} E\left[f(x)\right]$$

Therefore, the average of the minimums of replicated problems is an unbiased estimator of the left hand side if the batches of samples are i.i.d. Then the confidence interval for the lower bound is

$$v_{N,M} \pm t_{M-1,\alpha/2}\frac{S_{N,M}}{\sqrt{M}}$$

where, $v_{N,M} = \frac{1}{M}\sum_{m=1}^{M} v_N^{(m)}$, with $v_N^{(m)}$ denoting the solution of the m-th problem with sample size N, and

$$\frac{S_{N,M}}{\sqrt{M}} = \frac{1}{\sqrt{M(M-1)}}\sqrt{\sum_{m=1}^{M}\left(v_N^{(m)} - v_{N,M}\right)^2} \text{ , (m=1, 2, …, M).}$$

Then, the confidence interval of the optimality gap is

$$\left(0, \quad v_{N'} - v_{N,M} + t_{M-1,\alpha/2}\frac{S_{N,M}}{\sqrt{M}} + t_{N'-1,\alpha/2}\frac{S_{N'}}{\sqrt{N'}}\right)$$

When the above bounding techniques are applied to each NLP and MILP of the Outer Approximation method (Duran and Grossmann, 1986) for MINLPs, the confidence interval of the optimality gap of each NLP and MILP can be found. The sample sizes are increased if the interval of any optimality gap is not sufficiently small. The complete algorithm diagram can be found in Wei and Realff (2004). It has also been proposed that this rule to increase sample sizes may not be good because it is not necessary to make the confidence interval of a very bad solution sufficiently small. A different rule to increase the sample sizes, developed in Wei and Realff (2004), was to guarantee that the confidence intervals do not overlap. The probability of cutting off the optimal integer solution was also calculated, which can be used to adjust the sample sizes and other algorithm parameters.

Nonconvexity issue

The nonconvexities of the plastics separation problem mainly come from the bilinear terms of flow rate balances for the units and the mixers, and also the unit models. For the NLP subproblems, a global optimization solver, such as BARON (Sahinidis, 2000-2001), should be used, otherwise the convergence of Monte Carlo sampling can not be guaranteed and confidence interval of the upper bound is not valid. Unfortunately, only a local optimization NLP solver, SNOPT, is the only one available to the authors. Therefore, a global solution can not be guaranteed.

The nonconvexity issue has a more significantly impact on the MILP part, since the linearizations may cut off a significant part of the feasible region. Approaches to generate valid lower bounds include solution of a convexified MINLP (Lee and Grossmann, 2001; Kesavan et al, 2004) or MILP (Tawarmalani and Sahinidis, 2002, 2004). In this paper, a heuristic strategy (Viswanathan and Grossmann, 1990) with the aim of reducing the effect of nonconvexities on generating lower bounds in master problems is applied. This approach introduced slack variables in the master problem which has the following form

$$\begin{aligned}
&\min Z^K = \alpha + \sum_{k=1}^{K} w_p^k p^k + w_q^k q^k \\
&s.t. \quad \alpha \ge f\left(x^k, y^k\right) + \nabla f\left(x^k, y^k\right)^T \begin{bmatrix} x - x^k \\ y - y^k \end{bmatrix}, \qquad k = 1,\ldots,K \\
&\qquad T^k \nabla h\left(x^k, y^k\right) \begin{bmatrix} x - x^k \\ y - y^k \end{bmatrix} \le p^k, \qquad k = 1,\ldots,K \\
&\qquad \mathrm{g}\left(\mathrm{x}^k, y^k\right) + \nabla g\left(x^k, y^k\right)^T \begin{bmatrix} x - x^k \\ y - y^k \end{bmatrix} \le q^k, \qquad k = 1,\ldots,K \\
&\qquad \sum_{i \in B^k} y_i - \sum_{i \in N^k} y_i \le \left|B^k\right| - 1, \qquad k = 1,\ldots,K \\
&\qquad x \in X, y \in Y, p^k, q^k \ge 0
\end{aligned} \qquad \text{(MILP-APER)}$$

Where w_p^k, w_q^k are weights that are chosen sufficiently large; $T^k=\{\mathrm{sign}(\lambda_i^k)\}$ in which λ_i^k is the multiplier associated with the equation $h_i(x,y)=0$.

Lagrangian decomposition

The smaller NLP problems have the following form with the discrete variables already fixed.

$$\begin{aligned}
&\min_{x,z_i} \frac{1}{N} \sum_{i=1}^{N} f\left(x, z_i\right) \\
&s.t. \quad g_i\left(x, z_i\right) \le 0 \quad \mathrm{i} = 1,\cdots,\mathrm{N} \\
&\qquad x \in X, z_i \in Z
\end{aligned}$$

The problem has a block diagonal structure. Solving such a problem as a whole is time-consuming and sometimes intractable if the sample size, number of constraints and variables are very large.

However, the special structure of the problem can be exploited to decouple the scenarios and solve the problem in an iterative way until the decision variables x solved at each scenario converge to the same value. This can be done by first splitting the decision variable x into N variables x_i ($i=1, \ldots, N$)

and then applying Lagrangian Relaxation (Fisher, 1981; Guignard and Kim, 1987) to the copy constraints $x = x_i$. This is called Lagrangian Decomposition .

$$
\begin{aligned}
& \min_{x, x_i, z_i} \frac{1}{N} \sum_{i=1}^{N} f_i(x_i, z_i) \\
& s.t. \quad g_i(x_i, z_i) \le 0, \quad i = 1, \cdots, N \\
& \qquad x = x_i, \; i = 1, \cdots, N \\
& \qquad x, x_i \in X, z_i \in Z
\end{aligned}
$$

The Lagrangian of the above problem is

$$
L = \frac{1}{N} \sum_{i=1}^{N} f_i(x_i, z_i) + \sum_{i=1}^{N} \mu_i g_i + \sum_{i=1}^{N} \pi_i (x - x_i)
$$

Theoretically, if the problem is convex and the variables are continuous, the original problem is equivalent (in terms of the optimal objective value) to solving the following LD problem:

$$
\max_{\pi_i} \left[\min_{x_i, x} \left\{ \frac{1}{N} \sum_{i=1}^{N} f_i(x_i, z_i) + \sum_{i=1}^{N} \pi_i (x - x_i) \;\middle|\; g_i(x_i, z_i) \le 0, x, x_i \in X, z_i \in Z \right\} \right] \qquad \text{(LD)}
$$

However, a duality gap might exist in this case due to the non-convexities of the problem. Therefore the solution of LD provides a lower bound to the original problem. Any feasible solution to the original problem is an upper bound. Typically a sub-gradient method is used to update the multipliers to.

CASE STUDY

In this case study, the flow stream to be processed is a mixture of TV and Computer products. The components of a TV or a computer are assumed to be fixed, respectively. However, the fraction of TVs or Computers is uncertain, which makes the fraction of each component in the feed stream also a random number. The total feed flow rate is fixed at 3600 kg/hr (=1 kg/s) and the fraction of TVs has a normal distribution with mean 74% and standard deviation 17%. In TVs, HIPS is the dominant material, while in computers, ABS dominates. The data are shown in Table 1.

Table 1 Feed components and fractions (APC report, 2000)

		PE	HIPS	ABS	PPO	PC/ABS
Feed	Total: 3600 kg/ hr, TV (Mean: 74%; STD 17%) + Computer					
Components	For TV	5%	75%	8%	12%	0%
	For Computer	0%	5%	57%	36%	2%

The product prices are also uncertain and correlated, which are assumed to have normal distributions, with their respective mean and standard deviation and the correlation coefficient matrix shown in Table 2.

Table 2 Product price distribution

		PE	HIPS	ABS	PPO	PC/ABS
Price ($/kg)	Mean	0.4	0.6	0.6	1.5	1.5
	S.T.D.	0.02	0.04	0.04	0.1	0.1
	Correlation Coefficient	1	0.2	0.2	0.2	0.2
			1	0.5	0.3	0.3
				1	0.3	0.7
					1	0.4
						1

The following superstructure (Figure 1a,b) is used, which consists of 10 optional units (4 sink-float tanks (SF), 2 froth flotation tanks (FF), 2 free-fall electrostatic separators (FE) and 2 drum separators (DE)).

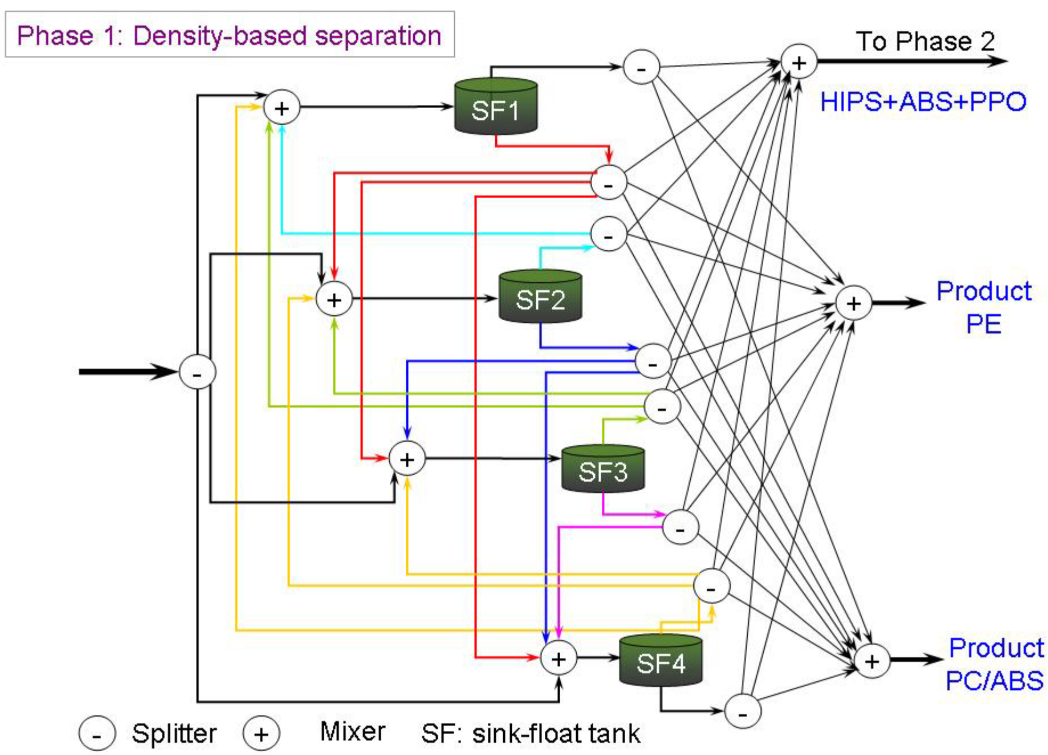

Figure 1 a   Phase 1 of plastics separation superstructure

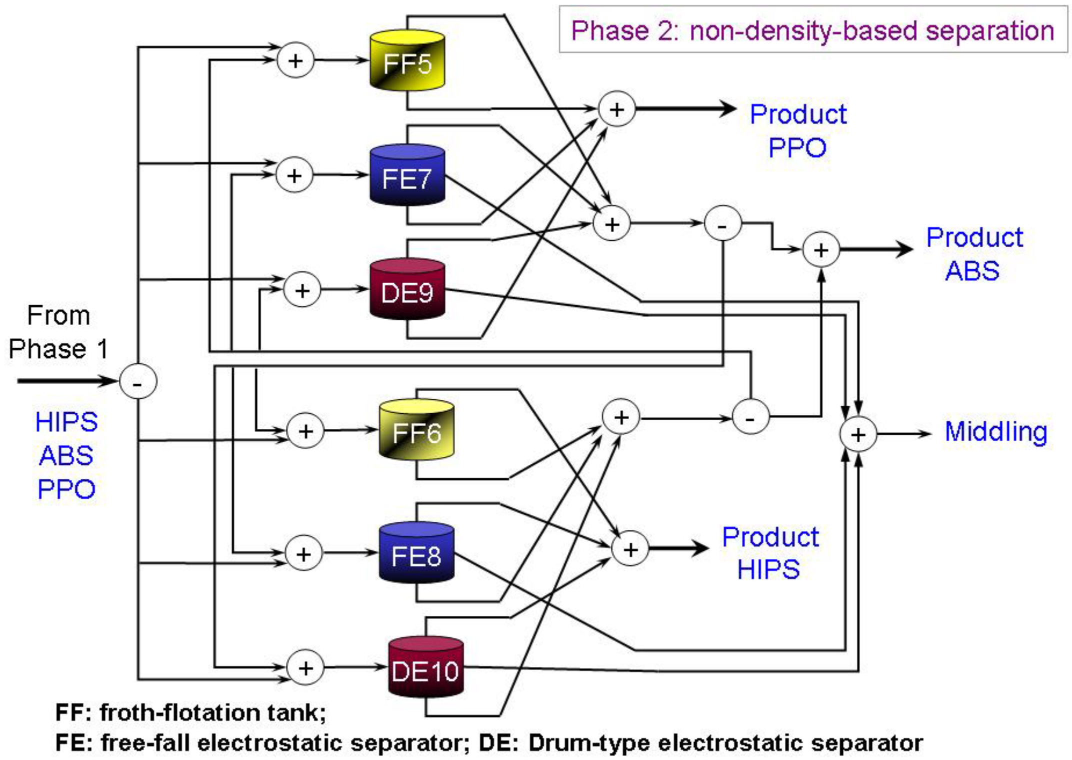

Figure 1b Phase 2 of plastics separation superstructure

The problem was solved with AMPL CPLEX 8.1 and SNOPT 5.3-4 on a PC with 2.53GHz CPU and 1G memory. All the objective values reported below have the units of million dollars. Starting with (0110111111) for the binary variables, the optimal solution was reached at the 2^{nd} iteration (0100001100) with an optimal objective value -3.622 (the negative sign is due to the transformation of the maximization problem into a minimization problem). One sink-float tank and two free-fall electrostatic separators are selected.

Lagrangian decomposition result

The Lagrangian decomposition problems can in general converge within 2 iterations with initial multiplier values 0.01. For example, at the first iteration, the lower bound generated by Lagrangian decomposition is -3.592 and the upper bound by the heuristic rule is -3.481. At the second iteration, the lower bound is -3.524 and the upper bound is -3.500. Since the relative difference of these two values is with 2%, the Lagrangian decomposition procedure is considered to have converged. Therefore, despite of the nonconvexities in the nonlinear problems, the duality gaps are negligible. If the initial multiplier values are increased to 0.1, the number of iterations for the convergence will increase to 6.

As a heuristic rule to find an upper bound, the variables x are fixed at the maximum of the $\hat{x}_i$ values found in step1 and then the problem is solved again. This heuristic rule can provide a tight upper bound and also the values of the decision variables for the larger NLP.

Comparison between the uncertain and the average conditions

The deterministic case under the average condition (feed fraction and product prices) is also solved and the optimal flowsheet is shown in Figure 2.

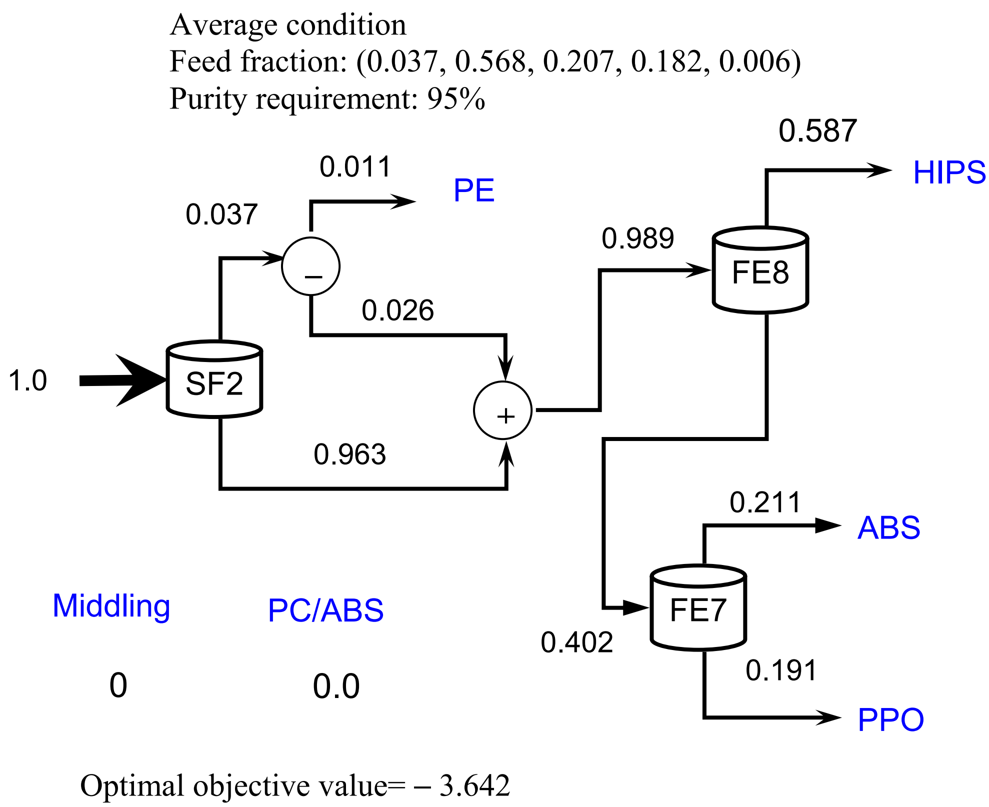

Figure 2 Optimal flowsheet of the deterministic case with 95% purity

The optimal objective value is -3.642, which is slightly better than that of the uncertain case, and the choices of the units are the same as in the uncertain case (Table 3). There is no difference between the uncertain and the average conditions in terms of the choice of units (i.e., flowsheet structure) because the variation in the feed composition has no influence on the unit separation efficiencies. However, from Table 3 it can be seen that the capacity of the second free-fall electrostatic separator designed under the average condition is under-designed.

Table 3 Comparison of the uncertain and average condition

	Under uncertainty	Average condition
Objective value	-3.622	-3.642
Choice of units	(0100001100)	(0100001100)
Capacity of unit 2	1.0	1.0
Capacity of unit 7	0.758	0.402
Capacity of unit 8	0.996	0.989

SAA Computational efficiency and the confidence of the solution

The computational time with the SAA method was 5 hours and 45 minutes. The computational saving is apparent compared with using a fixed sample size of 2000. Since at each OA iteration, the former requires solving 3400 single-size NLPs/MILPs (assuming the Lagrangian decomposition converges with 2 iterations for the first replication and 1 iteration for all other replications) and the latter requires solving 8000 single-size NLPs/MILPs (assume the Lagrangian decomposition converges with 2 iterations) .

Intuitively one would think that such a problem with a 10-dimensional uncertainty space should require very large sample sizes. However, our calculation result (Table 4) showed that the problem can be solved with small sample sizes (smaller sample size N=100, number of replications M=6, and larger sample size N'=2000) but still achieve high solution quality. The confidence intervals (99%) of the upper and lower bound at both iterations are less than 0.077, which is only around 2% of the optimal objective value. Of course, this result is problem-specific and can not be applied to other cases.

Table 4 Case study result – confidence intervals of optimality gaps (with N=100, M=6, N'=2000)

		Iteration 1 (0110111111)	Iteration2 (0100001100)
S-NLP	Mean of UB	-3.556	-3.660
	Variance of UB	0.0018	0.0023
L-NLP	Mean of UB	-3.545	-3.622
	Variance of UB	0.0891	0.0881
	Mean of UB gap	0.011	0.038
	CI of UB gap	**0.0708**	**0.103**
S-MILP	Mean of LB	-3.775	-3.675
	Variance of LB	4.09e-4	4.11e-4
L-MILP	Mean of LB	-3.753	-3.583
	Variance of LB	0.00893	0.00917
	Mean of LB gap	0.022	0.092
	CI of LB gap	**0.0576**	**0.0761**

CONCLUSION

This paper is the first systematic approach to solve a plastics separation design problem under uncertainty. The problem is formulated as a stochastic MINLP and solved by the previously proposed SAA method. The method can not only determine the appropriate sample sizes based on the solution quality requirement or vice versa, but also reduce the computational time by decoupling the scenarios using solutions from multiple problems with smaller sample size.

However, a drawback of the current SAA algorithm is its inability to handle nonconvexities. Future research includes development of a global optimization algorithm for stochastic nonconvex MINLPs .

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