Hybrid Intelligence Assisted Sample Average Approximation Method for Chance Constrained Dynamic Optimization

Xiaojun Zhou, *Member, IEEE,* Xiangyue Wang, Tingwen Huang, *Fellow, IEEE,* and Chunhua Yang, *Senior Member, IEEE*

***Abstract*—Realistic industrial process is usually a dynamic process with uncertainty. Chance constraints are applicable to industrial process modeling under uncertain conditions, where constraints cannot be strictly met, or need not be fully met. Therefore, chance constrained dynamic optimization (CCDO) formulation is available to address realistic industrial process issues. Because of the dynamic and uncertainty, chance constrained dynamic optimization problems (CCDOPs) arising from practical industries are hard to cope with. A novel CCDO method is proposed to resolve this issue, where an adaptive sample average approximation method, a control vector parameterization method, and a state constraint handling strategy are integrated. Specially, a hybrid intelligent optimization algorithm is introduced to realize a global and efficient optimization performance. The proposed method is applied to CCDOPs modified by dynamic optimization standard test functions and industrial experiments to demonstrate its effectiveness. The experimental results show that the proposed method has good performance in solving CCDOPs.**

***Index Terms*—Hybrid intelligence, data driven, sample average approximation, chance constrained optimization, dynamic optimization.**

I. Introduction

UNCERTAINTIES are inevitable in the realistic industries due to model simplifications, measurement errors, dynamically changing environments, etc. Over the past several decades, there has been growing interest in uncertain optimization. An optimal production strategy derived from the deterministic model may become infeasible owing to the fluctuation around nominal values [1]. In addition, realistic industrial process is generally dynamic. Therefore, the realistic industrial production process is usually a dynamic process with uncertainty. Due to the existence of uncertainties, dynamic and other complex characteristics, stability and reliability of production are seriously challenged. To realize consumption reduction and stable production, there has been growing interest in uncertain dynamic optimization.

Many actual industrial data have randomness, which, most of the time, can be described by probability distribution function. For instance, the error of data measurement usually obeys Gaussian distribution [2], and wind speed obeys Weibull distribution in wind power analysis [3]. In the case of industrial processes with random information, a stochastic programming model can be used. Chance constrained optimization is introduced in [4], which is an important branch of stochastic programming. The main feature of chance constrained optimization is that constraints under uncertain system are satisfied with a predefined probability level to ensure a certain degree of reliability. Moreover, a trade-off can be made between profitability and reliability of the system by adjusting the probability value in the chance constraint model [5]. In fact, the incomplete satisfaction of the constraint and the adjustable probability value mean that chance constraint is a kind of quantitative and controllable flexible constraint. The chance constraint model can be applied to the following two situations: (1) The fluctuation range of uncertain information is too large, so that constraint conditions cannot be strictly satisfied. (2) The boundary values of some constraints are most likely derived from production experience, and satisfying constraints strictly may be not necessary and incur high operating costs. Therefore, chance constraints are applicable to industrial process modeling under random conditions, where the constraints cannot be strictly met, or the constraints need not be fully met. The chance constraint model can be used to achieve a certain level of product specifications, availability of products, security, fault tolerance, risk aversion, etc [6]. Chance constrained optimization has been applied to optimal power flow [7], portfolio optimization [8], home energy management [9], process engineering [10], etc.

Chance constrained dynamic optimization problems (CCDOPs) aim to find a control trajectory so that the probability of the state trajectory within a certain process range is not less than a specified value. Chance constrained optimization is divided into two steps. First, the uncertainty problem is converted into a deterministic problem. Then, a deterministic optimization method is used to solve the deterministic problem obtained by first step. Note that, because the problems studied in this paper are dynamic, a discretization scheme is required to transform original infinite dimensional problem to a finite dimensional nonlinear programming (NLP) problem in the

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second step.

It is still a challenge to obtain a high-quality solution of CCDOPs efficiently for three main reasons. Firstly, most CCDOPs are too complex to be converted into a deterministic problem analytically, and therefore an alternative data-driven method will be used [11]. Secondly, dynamic optimization problems arising from industrial process usually involve the state constraints from production specifications, which is constrained at each time point. Thirdly, it is difficult to obtain satisfactory solutions efficiently for the resulting NLP problem, because such problems involving dynamic and uncertain systems are usually highly nonlinear [12].

At present, the deterministic transformation methods of chance constrained model mainly include analytical methods and data driven methods based on sampling approximation [13]. The analytical method of chance constraint deterministic transformation is only suitable for problems with some special structures, and usually requires multi-dimensional integration [14]. The data driven method based on sampling approximation is a more general efficient method. In data driven method, random samples are generated based on the probability density function (PDF) of uncertain information or taken from existing historical data to approximate the entirety of uncertain information. Once the samples are determined, the uncertain problem is transformed to a deterministic problem. The data driven methods do not depend on the problem structure and do not need calculate multi-dimensional integrals, which is versatile and efficient.

Sample average approximation (SAA) is a widely popular method for data driven decision under uncertainty [15]. SAA approximates the true distribution by sampling a part of data points, and places the same weight at each of the data points. In other words, a probability can be approximated by a frequency of satisfaction of constraint for a part of samples. Two advantages, asymptotic convergence and tractability underlie the popularity and practical success of SAA [15]. SAA has been widely applied to solve chance constrained optimization problems [16].

The major challenge of SAA method lies in the consumption and efficiency of calculation. A large sample size will cause a large computational cost, while a small sampling size will make the sampling approximation problem far from the original problem [17]. A standard SAA method generates only a single approximate problem with a sufficiently large sample size, which can guarantee a certain calculation accuracy but with low efficiency. To address this issue, some modifications have been investigated in SAA method. Retrospective-Approximation (RA) method is proposed in [18], where a sequence of approximate deterministic problems are solved with decreasing error and increasing Monte Carlo sample sizes. At early iterations of the algorithm, when the current iteration point is far from the optimal solution, there is no need to have high-precision approximation of original problem. Later iterations are effective because the initial solution to the later problem is likely to be close to the real solution, and not much effort is required to solve the later problem. In order to improve efficiency, an adaptive SAA method with adaptive sample size is adopted.

The deterministic problem obtained by SAA method is a dynamic optimization problem in this paper. A discretization scheme is required to transform original infinite-dimensional dynamic problem to a finite-dimensional NLP problem. Control vector parameterization (CVP) [19] method has been widely used to solve dynamic problem because of its easy implementation [20], [21]. It approximates the control trajectory with a set of parameterized basis functions, usually using uniform piecewise constant. State constraints are difficult to deal with because state trajectories have to be satisfied at every point in time. In general, there are two ways to consider state constraints: (1) satisfy the point constraint at discrete points, and (2) make the violation integral less than a small tolerance. However, the second way can only be applied to some problems with special structures. The first way is more versatile and has been widely applied to practical problems [16]. In this paper, considering the using of the CVP method, constraints at the time point of the CVP endpoint are taken into account.

After deterministic transformation, discretization and constraints handling, the existence of local optimal solutions and computational efficiency are still challenges for solving the resulting NLP problem. Owing to the complexity of actual industrial process, NLP problems arising in industrial process are multidimensional, nonconvex, nonlinear. Recently, intelligent algorithms such as genetic algorithm (GA) [22], particle swarm optimization (PSO) [23], differential evolution (DE) [24], have been well used to solve real-world optimization problems. Better global performance of these intelligent optimization algorithms has been found compared to gradient-based methods. An intelligent optimization algorithm named state transition algorithm (STA) [25] has been well applied in various fields and showed remarkable performance to solve nonconvex and multidimensional optimization problems. Although the convergence rate of the intelligent optimization algorithm is fast in the early iteration, the convergence rate declines obviously in the subsequent iteration when approaching the optimal solution. The gradient-based optimization methods have good convergence but are easy to fall into a local optimal solution. Therefore, a single intelligent algorithm is not enough to cope with the above NLP problem accurately and efficiently, but the advantages of gradient-based methods and intelligent algorithms can complement each other. In this paper, a hybrid intelligent optimization algorithm which combines the global search ability of STA and the fast convergence ability of gradient-based method is introduced to solve the resulting problem.

In this paper, a chance constrained dynamic optimization (CCDO) method is proposed for solving CCDOPs. The main contributions of this paper are given as follows. (1) An adaptive SAA is proposed to transform a CCDOP to a deterministic dynamic optimization problem. (2) A CVP method is used to transform the original problem into a finite dimensional NLP problem, and some special discrete points are selected to address the state constraint. (3) A hybrid intelligent optimization algorithm is introduced to solve the resulting NLP problem. (4) The proposed method is successfully applied to solve two CCDOPs arising from exothermal tubular plug flow reactor and copper removal process.

The rest of this paper is organized as follows. In Section 2, a CCDO method is proposed to solve CCDOPs. In Section 3, Two industrial experiments are conducted to demonstrate the effectiveness of the proposed method. Finally, the paper is concluded in Section 4.

II. Proposed Chance Constrained Dynamic Optimization Method

A general CCDOP can be illustrated in the form

$$\min_{\boldsymbol{u}(t)} \quad J = E(\phi(\boldsymbol{u}(t), \boldsymbol{x}(t), \boldsymbol{\xi})), \tag{1a}$$

$$\text{s.t. } \dot{\boldsymbol{x}} = f(\boldsymbol{u}(t), \boldsymbol{x}(t), \boldsymbol{\xi}) \tag{1b}$$

$$\Pr\{g_i(\boldsymbol{u}(t), \boldsymbol{x}(t), \boldsymbol{\xi}) \leq 0\} \geq \alpha_i, i = 1, 2, ..., n \tag{1c}$$

$$t \in [t_0, t_f], \boldsymbol{u} \in [\boldsymbol{u}^{\min}, \boldsymbol{u}^{\max}], \alpha_i \in [0, 1] \tag{1d}$$

where $\boldsymbol{u}(t)$ denotes the control vector and $\boldsymbol{x}(t)$ is the state vector. $\boldsymbol{\xi}$ is random vector with known PDF. n is the number of chance constraints. $\boldsymbol{u}^{\min}$ and $\boldsymbol{u}^{\max}$ are the the lower and upper bound of the control vector. t_0 and t_f are the initial and the final time. $g_i(\boldsymbol{u}(t), \boldsymbol{x}(t), \boldsymbol{\xi}), i = 1, 2, ..., n$ is inequality constraint, and $\Pr\{\cdot\}$ is the probability of satisfying the inequality constraints. E$(\cdot)$ is the expectation. α_i is a user-predefined probability level for ith inequality constraint.

In addition, in practical engineering, a very common form of inequality constraint is to restrict some state variables, which is called state constraints:

$$\Pr\{x_i^{\min} \leq x_i(t) \leq x_i^{\max}\} \geq \alpha_i, i = 1, 2, ..., n \tag{2}$$

Note that (2) denotes single chance constraints, and each of them specifies a probability level of keeping the state trajectory $x_i(t)$ between the bounds $x_i^{\min}$ and $x_i^{\max}$. Furthermore, $\Pr\{x_i^{\min} \leq x_i(t) \leq x_i^{\max}, i = 1, 2, ..., n\} \geq \alpha$ denotes joint chance constraints, and all specified state constraints are held at the same probability level simultaneously. Single chance constraints are more common in realistic industry [26], so we just consider single chance constraints in this paper.

The proposed CCDO method consists of three important parts. Firstly, an adaptive SAA method is investigated to transform the CCDOP into a deterministic dynamic optimization problem. Secondly, a CVP method is used to transform the original problem into a finite dimensional NLP problem, and some special discrete points are selected to address the state constraint. Thirdly, a hybrid intelligent optimization optimization algorithm is introduced to solve the resulting NLP problem. The proposed method is a data driven method based on sampling approximation, which doesn't depend on the problem structure and can be used to handle uncertainties with a variety of distributions. The framework of the proposed CCDO method is shown in Fig. 1.

A. Adaptive Sample Average Approximation Method

The main idea of the SAA method is to approximate the function value of the stochastic program by solving the problem with partial samples. By using SAA method, the

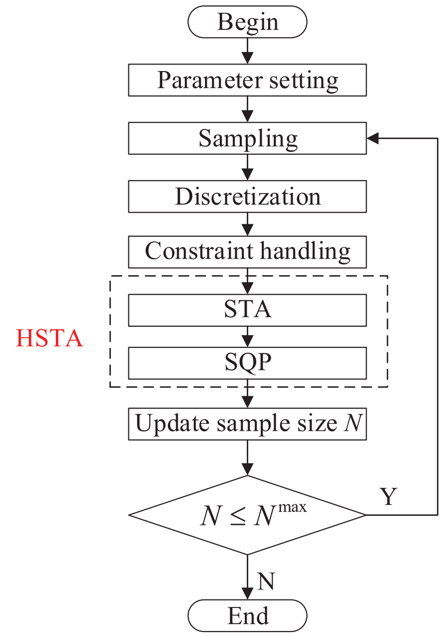

Fig. 1: Flow chart of the proposed method

chance constraint $\Pr\{g_i(\boldsymbol{u}(t), \boldsymbol{x}(t), \boldsymbol{\xi}) \leq 0\}$ can be approximated by a frequency of satisfying the constraint for samples $\{\boldsymbol{\xi}_1, \boldsymbol{\xi}_2, ..., \boldsymbol{\xi}_N\}$. Moreover, since the state $\boldsymbol{x}$ depends on control vector $\boldsymbol{u}$ and random vector $\boldsymbol{\xi}$, a more transparent expression of inequality constraints is $g_i(\boldsymbol{u}(t), \boldsymbol{\xi}) = g_i(\boldsymbol{u}(t), \boldsymbol{x}(t), \boldsymbol{\xi})$. The probability obtained by SAA is as follows

$$\Pr\{g_i(\boldsymbol{u}(t), \boldsymbol{\xi}) \leq 0\} = \frac{1}{N} \sum_{k=1}^{N} \mathbb{I}_{(-\infty,0]}(g_i(\boldsymbol{u}(t), \boldsymbol{\xi}_k)) \tag{3}$$

$$\mathbb{I}_{(-\infty,0]}(\zeta) = \begin{cases} 1, \zeta \leq 0 \\ 0, \zeta > 0 \end{cases}$$

where $\mathbb{I}_{(-\infty,0]}(\zeta)$ is indicator function. Then, the probability function can be described as

$$p_i(\boldsymbol{u}) = \Pr\{g_i(\boldsymbol{u}(t), \boldsymbol{\xi}) \leq 0\} \tag{4}$$

The potential difficulty associated with SAA is that frequency approximation of a probability requires a very large sample size. The standard SAA method can result in poor solution quality if the selected sample sizes are not large enough. However, for large sample sizes, the SAA method is not practical due to the significant computational effort required. In this paper, an adaptive SAA method generates a sequence of approximation problem with progressively increasing sample sizes, and then solves them with progressively decreasing tolerances. It is desirable to save the sampling effort when the current solution is far from the optimal solution, and increase the number of samples as the iteration approaches the optimal solution. The early iterations are efficient, because the small sample sizes ensure that not much computing effort in finding a coarse solution. Moreover, The later iterations are also efficient, because the starting solution for the approximation problem is probably close to the true solution, and not much effort is expended in solving approximation problems.

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There are various sample size growth rates [17], including exponential growth, polynomial growth and linear growth, for its better behavior, here we use the linear growth, $N_l = r \times N_{l-1}, l \geq 2$, where N_1 is the sample size of iteration 1 and r denotes growth rate of sample size. The tolerance is chosen to be proportional to $1/N_l$.

B. Discretization and State Chance Constraints Handling

After the model is transformed to a deterministic dynamic optimization problem by adaptive SAA method, discretization and state constraints handling for the deterministic dynamic optimization problem are discussed in this section. A discretization scheme is required to convert the dynamic problem with infinite dimension to a finite dimensional problem. By using control vector parameterization (CVP) method, the control variables are approximatively represented as piecewise polynomials, and then, the coefficients of polynomial which are finite dimension can be optimized. A uniform piecewise-constant parameterization scheme is introduced in this section, the control horizon will be divided by a set of knots $t_m, m = 0, ..., M$, where $M \geq 1$ and $t_0 < t_1 < ... < t_m < ... < t_M = t_f$. Then, the control trajectory over the whole span is approximated:

$$u(t) \approx \widetilde{u}(t) = \sum_{m=1}^{M} \delta_m(t)\omega_m, t \in [t_0, t_f], \tag{5}$$

$$\delta_m(t) = \begin{cases} 1 \,, t \in [t_{m-1}, t_m] \\ 0 \,, else \end{cases} \,, m = 0, ..., M$$

where $[t_{m-1}, t_m]$ is the mth control subinterval and ω_m is the constant control value on the mth subinterval. The original problem is transformed into a parameter selection problem.

To address state constraint, discretization points constraints in the endpoint of each subintervals obtained by CVP method are taken into account to approximate the state constraint, shown as follows:

$$p_i(\boldsymbol{\omega}) = \Pr\{x_i^{\min} \leq x_i(t) \leq x_i^{\max}\} \geq \alpha_i, \tag{6}$$
$$i = 1, 2, ..., n, t \in \{t_1, ..., t_m, ..., t_M\}$$

where $t_1, ..., t_m, ..., t_M$ are the endpoints of each subintervals, control values $\boldsymbol{\omega} = [\omega_1, \omega_2, ..., \omega_M]$ are the decision variables. Schematic diagram of CVP and constrained points are shown in Fig. 2.

Penalty function method is one of the most common methods to deal with constraints in optimization problems. After control parameterization, a penalty function is used to generate a new cost function:

$$J_1(\boldsymbol{\omega}) = J(\boldsymbol{\omega}) + \rho \sum_{i=1}^{n} \sum_{j=1}^{M} \max\{\alpha_i - p(\boldsymbol{\omega}), 0\} \tag{7}$$

where n is the number of the state constraints, M is the number of the constrained points for ith state constraint, $\rho > 0$ is a penalty factor.

CCDOP becomes an unconstrained NLP problem after constraints handling. Note that the number of chance constraints is related to the number of discrete nodes, which can lead to intensive calculations.

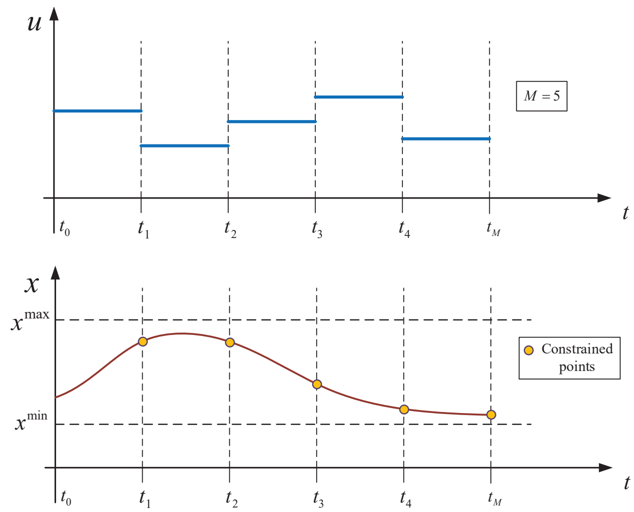

Fig. 2: Schematic diagram of CVP and constrained points

C. Hybrid Intelligent Optimization Algorithm

STA is an intelligent optimization algorithm, which has been applied in many complex industrial problems due to its remarkable global search capability [25]. Therefore, STA has advantages in solving non-convex NLP problems. In STA, a solution to an optimization problem is considered as a state, and the update process of the solution is considered as a state transition process. Four special state transformation operators are designed to search for optimal solution in STA. The state transition process can be described in a unified framework:

$$\begin{cases} \boldsymbol{x}_{k+1} = A_k \boldsymbol{x}_k + B_k \boldsymbol{u}_k \\ y_{k+1} = f(\boldsymbol{x}_{k+1}) \end{cases} , \tag{8}$$

where $\boldsymbol{x}_k \in \Re^n$ represents a solution; $\boldsymbol{u}_k$ is the function of $\boldsymbol{x}_k$ and historical solutions; A_k and B_k are state transition matrices; $f(\cdot)$ is the evaluation function, and y_{k+1} is the evaluation value of solution $\boldsymbol{x}_{k+1}$.

Although STA shows good global search capability, the convergence rate of such intelligent optimization method declines rapidly as the iteration progresses. Meanwhile, gradient-based algorithms converge quickly in local search. Therefore, in order to combine the global search capability of STA and the fast convergence ability in local search of the gradient-based algorithm, a hybrid intelligent optimization algorithm, named HSTA, is introduced. In the first phase aiming to find a rough global solution position. The second phase aims to speed up the convergence, where a gradient-based method sequential quadratic programming (SQP) will be adopted.

D. Proposed Chance Constrained Dynamic Optimization Method Procedure

The pseudocode of the proposed CCDO method is shown in Algorithm 1. The maximum sample size $N^{\max}$ is designed to guarantee a certain calculation accuracy, meanwhile, avoid solving problems with too large samples. The criterion $\left|\frac{J_l - J_{l-1}}{J_{l-1}}\right| \leq \varepsilon_s$ means that the convergence rate is going to slow down. It implies that it's time to use a fast convergence algorithm SQP in the base of solution obtained by STA.

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Algorithm 1 Pseudocode of the proposed CCDO method

Set maximum sample size $N^{\max}$, sample size growth factor r, global search termination tolerance ε_s, initial sample size N_1;
Set sample iteration $l = 1$;
Generate a set of random samples with sample size N_1;
Obtain a set of subintervals by CVP method;
Initialize M-dimensional solution $\boldsymbol{\omega}_1$ randomly;
while $N_l \le N^{\max}$ **do**
  Transform state chance constraint (2) to discrete time points constraint (6);
  Calculate the approximate probability value $p(\boldsymbol{\omega})$ in (6) by approximate frequency (3) with random samples $\{\boldsymbol{\xi}_1, \boldsymbol{\xi}_2, ..., \boldsymbol{\xi}_{N_l}\}$;
  Transform constrained NLP problem to unconstrained one (7) by penalty function;
  Obtain an approximate optimal solution $\boldsymbol{\omega}_l$ by STA with initial solution $\boldsymbol{\omega}_l$;
  while $\left|\frac{J_l - J_{l-1}}{J_{l-1}}\right| \le \varepsilon_s$ **do**
    Obtain the optimal solution $\boldsymbol{\omega}_l^*$ by solving (7) with SQP and initial solution $\boldsymbol{\omega}_l$;
    Let $l = l + 1$;
    Update sample size $N_l = r \times N_{l-1}$;
    Generate a set of random samples with sample size N_l;
  end while
end while

Note that, the step tolerance of SQP decreases as the sample iteration progresses, which is chosen to be proportional to $1/N_l$. In the next procedure, optimization will be made with larger sample size in the base of the previous generations optimal solution.

$$\sup |p_{N_l}(x) - p(x)| \to 0, w.p.1, \quad as\, N_l \to \infty. \tag{9}$$

As shown in (9), by the law of large numbers, we have that, p_{N_l} converges w.p.1 to $p(x)$. It is worth noting that a gradient-based algorithm is used in the second phase of HSTA, and it can guarantee that the algorithm will converge to a local minimum. Sampling precision and convergence analysis of an adaptive SAA method with gradient-based algorithms have be given in [17], which are also suitable for the proposed method.

III. Experiments and Discussion

In order to verify the effectiveness of the proposed CCDO method, we conduct two class of experiments: (1) CCDO problems modified by dynamic optimization standard test functions; (2) industrial experiments. All calculations are carried on MATLAB (Version R2016b) software platform using 2.3GHz Intel i5 PC with 8G RAM. Initial sample size N_1 and maximum sample size $N^{\max}$ are user-specified depending on problem. The parameter setting is shown in Table I.

TABLE I: The parameter setting of experiments

Parameter	Value
Sample size growth factor r	2
Termination parameters global search termination tolerance ε_s	1×10^{-2}
The number of piecewise interval	5
Probability level α	0.9

A. CCDO Problems Modified by Dynamic Optimization Standard Test Functions

Tubular batch reactor (TBR) considered in [27] and van der pol oscillator (VDPO) considered in [28] are dynamic optimization standard test functions, in which two uncertain parameters are added to make them become CCDO problems.

$$\min_{\boldsymbol{u}(t)} \ J(\boldsymbol{u}(t)) = -x_2(t_f), \tag{10a}$$
$$\text{s.t. } \dot{x}_1 = -\xi_1 x_1 (u + \frac{u^2}{2}) \tag{10b}$$
$$\dot{x}_2 = \xi_2 u x_1 \tag{10c}$$
$$\Pr(x_1(t) \ge 0.2) \ge \alpha \tag{10d}$$
$$\boldsymbol{x}(t_0) = [1, 0] \tag{10e}$$
$$0 \le u(t) \le 5, \tag{10f}$$
$$t_0 = 0, t_f = 1 \tag{10g}$$

where ξ_1, ξ_2 are both uncertain parameters with uniform distributions U(0.8, 1).

$$\min_{\boldsymbol{u}(t)} \ J(\boldsymbol{u}(t)) = x_3(t_f), \tag{11a}$$
$$\text{s.t. } \dot{x}_1 = \eta_1 x_1 (1 - x_2^2) - x_2 + u \tag{11b}$$
$$\dot{x}_2 = \eta_2 x_1 \tag{11c}$$
$$\dot{x}_3 = x_1^2 + x_2^2 + u^2 \tag{11d}$$
$$\Pr(x_1(t) \ge -0.4) \ge \alpha \tag{11e}$$
$$\boldsymbol{x}(t_0) = [0, 1, 0] \tag{11f}$$
$$-0.3 \le u(t) \le 1, \tag{11g}$$
$$t_0 = 0, t_f = 5 \tag{11h}$$

where η_1 is a normal distribution N(1, 0.1), and η_2 is a uniform distribution U(0.9, 1).

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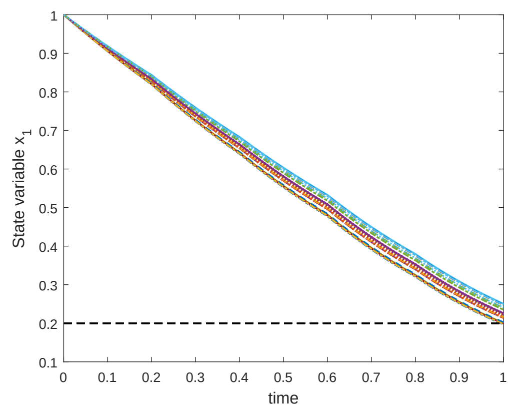
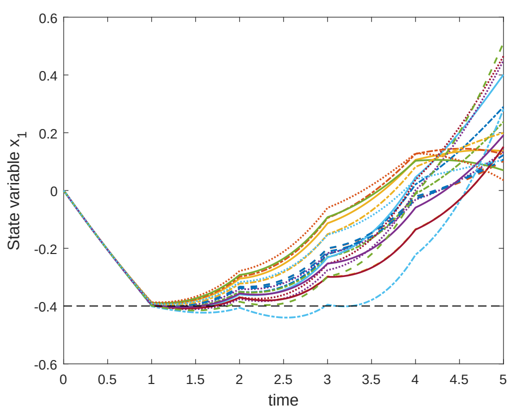
TABLE II: Results of standard test functions solved by proposed method

Problem	Method	G	J
TBR	Proposed method	0	3.5705
VDPO	Proposed method	0	0.5123

The results of standard test functions solved by proposed method are shown in Table II. The state profiles of standard test functions obtained by proposed method are illustrated in Fig. 3. The state profiles are obtained by Monte Carlo simulation with 20 samples. $G = 0$ in Table II and state profiles show that the outputs can meet the constraints well, which indicate the effectiveness of the proposed method.



(a) State profiles of TBR



(b) State profiles of VDPO

Fig. 3: State profiles of standard test functions

B. Industrial Experiments

1) Case I: Exothermal Tubular Plug Flow Reactor (ETPFR): The first industrial experiment involves a exothermal tubular plug flow reactor operating under steady-state conditions proposed in [29]. An exothermic reaction takes place inside the reactor, while a surrounding jacket removes the heat. The aim is to obtain an optimal jacket temperature profile profile along the reactor. The objective is to minimize the outlet reactant concentration which is associated with the maximization of the conversion. Due to the changeable production conditions and complex mechanisms, there exist uncertainties in the exothermal tubular plug flow reactor, which affect the stability and reliability of production. For instance, heat transfer coefficient β is usually difficult to measure and varies along the reactor owing to local fouling on the reactor wall. In general, the temperature limits of the reactor are derived from estimates of production experience and do not need to be fully met. Therefore, optimal control problem arising from ETPFR can be modeled as a chance constrained optimization problem. The model of ETPFR can be described:

$$\min_{u(z)} \quad J(\boldsymbol{u}(z)) = C_{in}(1 - x_1(L)), \tag{12a}$$

$$\text{s.t.} \quad \frac{dx_1}{dz} = \frac{\alpha_{kin}}{v}(1 - x_1)e^{\frac{\gamma x_2}{1+x_2}} \tag{12b}$$

$$\frac{dx_2}{dz} = \frac{\alpha_{kin}}{v}(1 - x_1)e^{\frac{\gamma x_2}{1+x_2}} + \frac{\beta}{v}(u - x_2) \tag{12c}$$

$$\boldsymbol{x}(0) = [0, 0] \tag{12d}$$

$$\Pr\left(\frac{T^{\min} - T_{in}}{T_{in}} \le x_2(z) \le \frac{T^{\max} - T_{in}}{T_{in}}\right) \ge \alpha \tag{12e}$$

$$\frac{T_w^{\min} - T_{in}}{T_{in}} \le u(z) \le \frac{T_w^{\max} - T_{in}}{T_{in}}, \tag{12f}$$

$$z \in [0, L] \tag{12g}$$

where T and T_w denote temperature of reactor fluid and jacket fluid. C indicates the reactant concentration. v is reactor fluid superficial velocity, L is reactor length, and z denotes spatial coordinate. State variables $x_1 = (C - C_{in})/(C_{in})$ and $x_2 = (T - T_{in})/T_{in}$ indicates dimensionless of reactant concentration C and reactor temperature T. Control variable $u = (T_w - T_{in})/T_{in}$ indicates dimensionless of jacket fluid temperature T_w. Superscript $\min$ and $\max$ denote values at its lower bound and upper bound. Subscripts in denotes value at the inlet. Two uncertain parameters, the kinetic coefficient α_{kin} of the reaction and the heat transfer coefficient β are taken into consider according to [30], and the values of them are shown in Table III. The other working condition can be shown in Table IV. Initial sample size N_1 and maximum sample size $N^{\max}$ are set as 20 and 640.

TABLE IV: The working condition of ETPFR

Parameter	Unit	Value
Inlet fluid temperature T_{in}	K	340
Minimum temperature of reactor fluid $T^{\min}$	K	280
Maximum temperature of reactor fluid $T^{\max}$	K	400
Minimum temperature of jacket fluid $T_w^{\min}$	K	280
Maximum temperature of jacket fluid $T_w^{\max}$	K	400
Reactor fluid superficial velocity v	m/s	0.1
Inlet reactant concentration C_{in}	mol/L	0.02
Intermediate parameter γ	–	16.5
Intermediate parameter δ	–	0.25
Length of the reactor L	m	1

2) Case II: Copper Removal Process (CRP): The CRP aims to remove copper ions from zinc sulfate solution by adding zinc powder into reactors, which is shown as Fig. 4.

TABLE III: The parameters of uncertain variables in the ETPFR

Parameter	Expected value	Standard deviation	Correlation matrix
Reaction kinetic coefficient α_{kin}	0.0581 s^{-1}	0.00581	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
Heat transfer coefficient, β	0.2 s^{-1}	0.02	

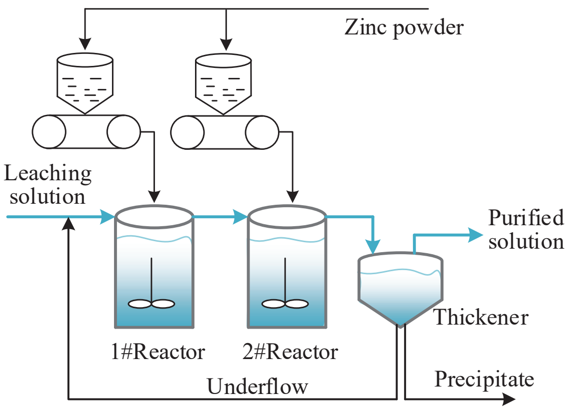


Fig. 4: Schematic diagram of the CRP

Due to the changeable production conditions, diverse mineral resources and complex reaction mechanism, it is difficult to maintain production stability and reliability. This paper mainly considers the uncertainty of inlet solution flow rate Q, returned underflow rate q and inlet copper ions concentration x_0 in the CRP, and the values of uncertain parameters are shown in Table V. Practical experience shows that the output copper ions concentration between 0.2g/l and 0.4g/l can promote the reaction of cobalt removal in the next process. But this range 0.2g/l-0.4g/l is based on production experience and does not need to be strictly met. Furthermore, the fluctuation of flow rate and inlet ions concentration is too large to strictly stabilize the copper ion concentration at the outlet at 0.2g/l-0.4g/l. Therefore, CRP under uncertainty can be modeled as a chance constraint optimization problem. The chance constrained optimal control problem of CRP can be described:

TABLE VI: The working condition of CRP

Parameter	Unit	Value
Solution volume V	m^3	100
Initial #1 concentration of outlet copper ions $\boldsymbol{x}_1(t_0)$	g/L	0.7
Initial #2 concentration of outlet copper ions $\boldsymbol{x}_2(t_0)$	g/L	0.4
Rate of zinc powder addition, u_i	kg/h	0-500
Desired concentration of outlet copper ions x_2	g/L	0.2-0.4

$$\min_{\boldsymbol{u}(t)} \quad J(\boldsymbol{u}(t)) = \int_{t_0}^{t_f} (u_1(t) + u_2(t))dt, \tag{13a}$$

$$\text{s.t. } \dot{x}_1 = \frac{Q}{V}x_{in} - \frac{Q+q}{V}x_1 - (k_1u_1 + k_2)x_1 \tag{13b}$$

$$\dot{x}_2 = \frac{Q+q}{V}x_1 - \frac{Q+q}{V}x_2 - (k_1u_1 + k_3)x_2 \tag{13c}$$

$$\boldsymbol{x}(t_0) = [x_1(t_0), x_2(t_0)] \tag{13d}$$

$$\Pr(C^{\min} \leq x_2(t) \leq C^{\max}) \geq \alpha \tag{13e}$$

$$u_i^{\min} \leq u_i(t) \leq u_i^{\max}, i = 1,2 \tag{13f}$$

$$t \in [t_0, t_f] \tag{13g}$$

where (13b) and (13c) are the differential algebraic equation constraint, $\boldsymbol{u}(t)$ denotes the control vector and $\boldsymbol{x}(t)$ denotes the state vector, $\boldsymbol{x}(t_0)$ is the initial state at time t_0, and t_f is the final time. Control variables $u_i, i = 1,2$ indicate the zinc powder addition rate of the ith reactor. State variables $x_i, i = 1,2$ indicate the outlet copper ions concentration of the ith reactor. $u_i^{\min}$ and $u_i^{\max}$ are the the lower and upper bound of zinc powder addition rate. $C^{\min}$ and $C^{\max}$ are the lower and upper bound of outlet copper ions concentration. $k_i, i = 1,2,3$ denotes kinetic parameters, which can be found in [31]. V, Q and q indicate the active volume of reactor, inlet solution flow rate and returned underflow rate respectively. Initial time $t_0 = 0$ and the final time $t_f = 2$. Other working condition can be shown in Table VI. Initial sample size N_1 and maximum sample size $N^{\max}$ are set as 100 and 1600.

3) Experimental Results: Comparison results of different NLP solvers are shown in Table VII, where Time denotes time consumption, and $G = \sum_{j=1}^{M} \max\{\alpha - p(\boldsymbol{u}), 0\}$ denotes gross constraint violation. It can be seen that high quality solutions can be obtained by using STA independently, but the computation cost is expensive. Although the calculation cost of using SQP independently is small, it is easy to fall into the local optimal solution. HSTA can obtain high-quality solutions with little time cost, which denotes hybrid intelligent optimization can combine the advantages of STA and SQP. Comparison results between SAA method with adaptive strategy and without adaptive strategy are shown in Table VIII. It can be seen that the adaptive SAA can obtain the same quality solution as SAA without adaptive strategy, but it is more efficient than the SAA without adaptive strategy. The adaptive SAA can increase the sample sizes along the algorithm, so that sampling effort is not wasted at the initial iterations. Moreover, later iterations of adaptive SAA are effective because the initial solution to the later problem is likely to be close to the real solution, and not much effort is required to solve the later problem.

The optimal control trajectory and state profiles of ETPFR and CRP obtained by proposed method are illustrated in Fig.

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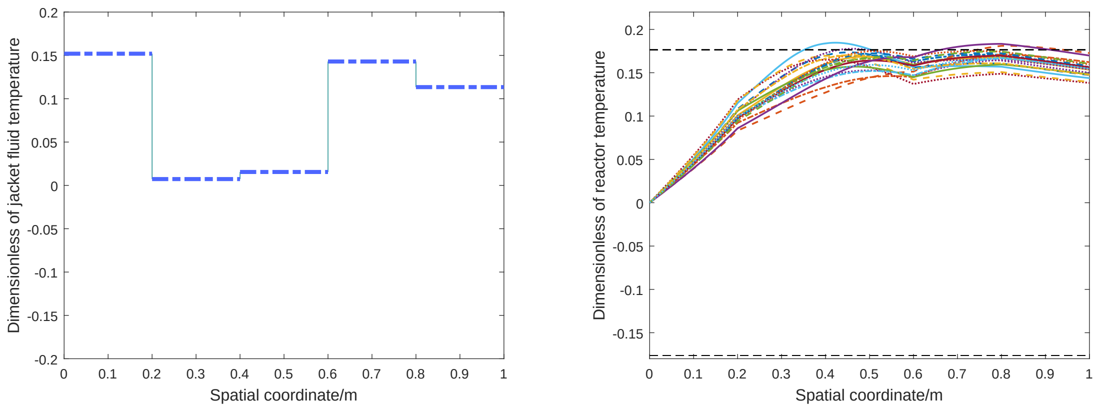
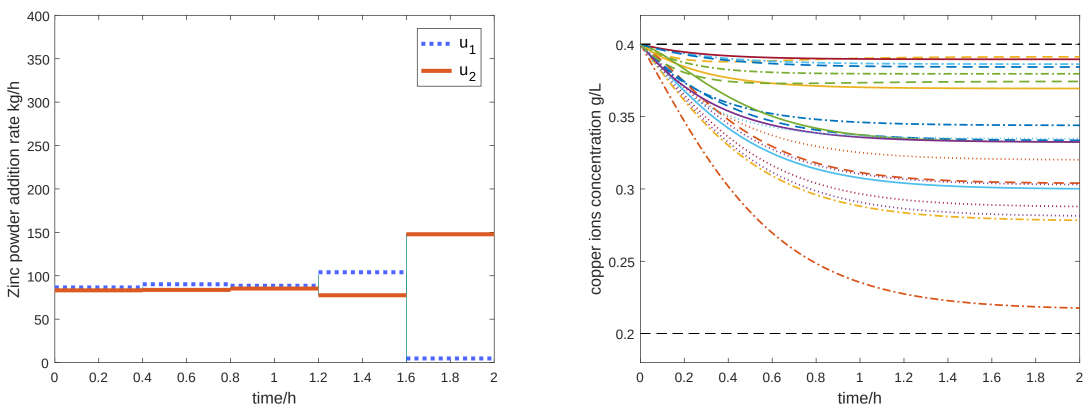
TABLE V: The parameters of uncertain variables in the CRP

Parameter	Expected value	Standard deviation	Correlation matrix		
Flow rate of leaching $ZnSO_4$ solution, Q	$187.00\ \mathrm{m^3/h}$	23.375	1	0.1489	0.0695
Flow rate of underflow, q	$12.56\ \mathrm{m^3/h}$	1.507	0.1489	1	0.2324
Inlet copper ions concentration, x_{in}	$1.22\ \mathrm{g/L}$	0.158	0.0695	0.2324	1



(a) Control trajectory (b) State profiles

Fig. 5: Optimal results of ETPFR



(a) Control trajectory (b) State profiles

Fig. 6: Optimal results of CRP

5 and Fig. 6, respectively. The state profiles are obtained by Monte Carlo simulation with 20 samples. $G = 0$ in Table VIII and state profiles show that reactor temperature of ETPFR and the outlet copper ions concentration of CRP can meet the production constraints well, and indicate the effectiveness of the proposed method.

To further verify the performance of the proposed CCDO method, comparative studies are conducted to analyze the objective functions and constraint violations obtained by performing the proposed method and other typical techniques. For example, conditional value-at-risk (CVaR) approximation method reported in [32], scenario approach (SA) reported in [33], and standard SAA reported in [34]. Comparison results of different chance constrained optimization method are shown in Table IX. We can see that the results from the proposed

TABLE VII: Comparison results of different NLP solvers

Problem	NLP solver	G	J	Time(s)
ETPFR (min)	STA	0	3.589×10^{-4}	411
	SQP	0.0953	1.5×10^{-3}	94
	HSTA	0	3.299×10^{-4}	182
CRP (min)	STA	0	382.0126	56
	SQP	1.715	461.7556	4
	HSTA	0	334.5470	32

method are much better than the results from other chance constrained optimization method, which verifies the effectiveness of the proposed method. The results show that CVaR approximation, SA and the proposed method can be feasible

TABLE VIII: Comparison results between SAA method with adaptive strategy and without adaptive strategy

Problem	SAA method	G	J	Time(s)
ETPFR (min)	Without adaptive	0	3.709×10^{-4}	240
	With adaptive	0	3.299×10^{-4}	182
CRP (min)	Without adaptive	0	334.7527	49
	With adaptive	0	334.5470	32

TABLE IX: Comparison results of different chance constrained optimization (CCO) method

Problem	CCO method	G	J
ETPFR (min)	CVaR	0	2.9×10^{-3}
	SA	0	1.1×10^{-3}
	Standard SAA	0	2.1×10^{-3}
	Proposed method	0	3.3×10^{-4}
CRP (min)	CVaR	0	448.8334
	SA	0	378.3635
	Standard SAA	1.1838	409.4292
	Proposed method	0	334.5470

for two industrial experiments, but standard SAA obtain an infeasible solution when solving CRP. As can be seen from Table IX, the proposed method can generally perform better than CVaR and SA in terms of achieving a smaller cost value. The CVaR approximation replaces indicator function with a conservative piecewise convex function in probability calculation. The SA employs a set of samples' constraints for the stochastic variables so as to approximately replace the probabilistic constraints. Therefore, the conservatism of CVaR approximation and SA are usually high and difficult to be controlled. In other words, CVaR and SA have greater conservatism compared with the proposed method, so the cost value is higher. Standard SAA does not have a conservative strategy, so the local solution is easily infeasible. The proposed method performs better global ability, and less conservatism.

In addition, a user-defined compromise between profitability and reliability that can be determined by the choice of α. It is easy to see that cost increases as reliability increases. The relationship between profitability and reliability of CRP

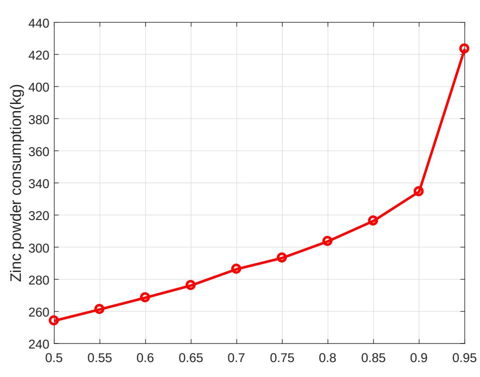


Fig. 7: Relationship between the probability level (α) and zinc powder consumption

is shown in Fig. 7, so that decision-makers can make tradeoffs between profitability and reliability.

IV. Conclusion

In this study, a novel CCDO method is proposed. First, the original uncertain dynamic problem is converted to a deterministic problem based on an adaptive SAA method, which can adjust sample size adaptively. Second, the dynamic infinite dimensional problem is transformed to a finite dimensional NLP problem by using CVP method, and constrained points in the endpoint of each discrete subintervals are taken into account to approximate the state constraint. Third, a hybrid intelligence optimization algorithm, which combines STA and SQP method, is introduced to solve the resulting problem globally and efficiently. Experimental results show that the proposed method has good performance in solving CCDOPs. Furthermore, the relationship between profitability and reliability is constructed, which can provide decision support for actual industrial process. In the future, we will continue to solve the CCDOPs with joint chance constraints.

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