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Dynamic Optimization for Copper Removal Process with Continuous Production Constraints

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***Abstract*—The copper removal process (CRP) aims to reduce the copper ion concentration in zinc sulphate solution to a specific range by zinc addition. The satisfaction of production constraints and minimization of zinc consumption are vital but difficult to achieve. In this paper, the dynamic optimization for CRP is conducted for optimal zinc control trajectory design considering constraints at least cost. First, a dynamic optimization problem with both state and control constraints is constructed for CRP. Then, a constrained dynamic optimization method is proposed, where a wavelet-based control parameterization method and a smooth penalty method are adopted. Specially, a hybrid optimization strategy is proposed to achieve a robust and efficient optimization performance. Numerical experiments are provided to illustrate the effectiveness of the proposed method. Results show that the proposed method can produce not only the optimal control trajectory with a qualified outlet ion concentration, but also the less zinc consumption.**

***Index Terms*—Copper removal, dynamic optimization, control vector parameterization, inequality constraints, state transition algorithm.**

I. Introduction

PURIFICATION of zinc sulfate solution is indispensable in zinc hydrometallurgy, since the existence of impurity ions, such as copper, cobalt and nickel, may cause the problems of corrosion, product purity and work hygiene [1]. As the first stage of solution purification, copper removal process (CRP) is of considerable importance, which serves to reduce the copper ion concentration to a precise range by zinc addition for facilitating the downstream cobalt removal process [2]. It is difficult for operators to make appropriate operation to meet the strict requirements of process output, due to the intricate reaction mechanism and the off-line ion concentration measurement. An extremely conservative strategy commonly used in practice usually leads to not only excessive zinc powder consumption but also insufficient outlet copper ions. In order to find an optimal control trajectory with less zinc consumption within a qualified ion concentration, the dynamic optimization of CRP was constructed (see [3] and the references therein).

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The optimization problem arising in CRP can be constructed to a dynamic optimization problem (DOP), whose objective is to find a time-varying control trajectory corresponding to reducing production costs for a given process time. More significantly, the optimization is performed in the presence of various production constraints, i.e., the intrinsic constraints imposed by the dynamic system differential equations, the input constraints dictated by equipment requirements, and the state-dependent constraints stemming from safety and operability consideration [4].

It is still a challenge to obtain a high-quality solution of DOPs efficiently, especially when the problem formulation contains continuous inequality constraints, for three primary reasons. Firstly, most constrained DOPs are much too complex to be soluble analytically [5], and therefore they can only be solved by numerical method with additional parameterization operation. Secondly, the state trajectory subjects to constraints at every time point, and thus an uncountable number of point constraints need to be satisfied simultaneously. Thirdly, even for the problem without constraints, the solution quality obtained by numerical method is not always satisfactory, because such optimization problems involving dynamic systems arising in industrial process are usually highly nonlinear, multidimensional and multimodal [6].

Control vector parameterization (CVP) [7] method is widely used in numerical method to reduce the original infinite-dimensional problem to a finite-dimensional non-linear programming (NLP) problem. It only approximates control trajectory using a finite number of decision variables, commonly with a uniform piecewise-constant approximation scheme. However, an uniform parameterization grid has a dilemma that the solution quality is strongly dependent on the parameterization resolution of the control trajectory. The higher resolution brings more accurate approximation while takes significantly higher computational cost [8]. Moreover, high-frequency control due to the high resolution will make it difficult and expensive to implement in practice. In order to make a tradeoff among approximation, optimization and operation, a wavelet-based CVP method based on adaptive refinement strategy suggested in [9] is adopted in this paper to reflect the optimal control trajectory structure with less decision parameters.

To deal with the continuous inequality constraint, some approaches have been studied in the framework of CVP method. One traditional approach introduces a slack variable to transform original problem with a state inequality constraint into an unconstrained one of increased dimension [10].

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However, it can only be applied to problems with special structures. Another method, called exact penalty method, is more versatile and has been successfully applied to a wide variety of practical problems. It involves appending the constraint violation to the cost function as a penalty term and then constructing an unconstrained penalty problem. Since the exact penalty functions are nondifferentiable, a smooth technique is introduced to approximate the penalty operator for facilitating the subsequent optimization [11].

After parameterization and constraint handling, the existence of suboptimal local minima is still a troublesome problem when solving DOPs [12]. The characteristics of highly nonlinear, multidimensional and multimodal make gradient-based optimization methods struggle to handle [13], which have good convergence in local search. To address this issue, a stochastic global optimization algorithm named state transition algorithm (STA) [14] is introduced, and its excellent global performance for solving unconstrained dynamic optimization problems has been reported. Although STA converges fast in the initial stage, its convergence speed decreases considerably in later iterations when reaching a near-optimal solution. In this paper, it is desirable to investigate a hybrid optimization method which combines the global search ability of STA and the local search ability of gradient-based method.

In this paper, we intend to find a zinc addition trajectory for a given operating time such that the outlet copper ion concentration can keep in a desirable range at the most economical cost. The main contributions of this paper are summarized as follows. (1) A dynamic optimization problem is constructed for CRP to find the optimal control trajectory of zinc addition for a given time, with considerations of production constraints. (2) A constrained dynamic optimization method is proposed to solve the DOPs with continuous state constraints, based on the wavelet-based CVP method and smooth penalty method. Specially, a hybrid optimization strategy combined STA and gradient-based method is investigated to obtain a robust and efficient optimization performance. (3) The proposed method is successfully applied to solve the constrained DOP arising in CRP. The dynamic optimization framework of CRP is shown in Fig.1.

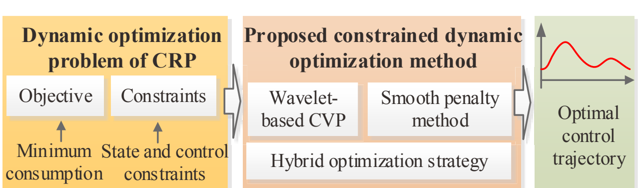

Fig. 1: The dynamic optimization of CRP

The remainder of this paper is organized as follows. In Section 2, after process analysis and modeling, a dynamic optimization problem with inequality constraints is constructed for CRP. In Section 3, a dynamic optimization method is proposed for solving constrained DOPs. Section 4 demonstrates the effectiveness of the proposed method. Finally, the conclusion is drawn in Section 5.

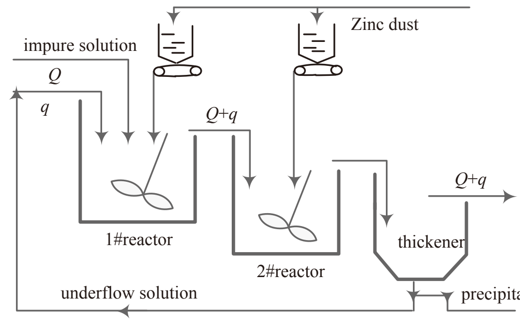

Fig. 2: Schematic diagram of the CRP

II. Dynamic Optimization Problem of CRP

A. Process Description and Modeling

In CRP, the separation of copper from the leaching $ZnSO_4$ solution is carried out with two cascaded reactors, shown as Fig. 2. It is observed that the leaching solution is fed into two reactors continuously and then sent to a thickener for solid-liquid separation. The first reactor acts as main reactor responsible for the deposition of most of copper ions, while the second reactor serves as auxiliary for fine tuning the outlet concentration. Zinc serves as the cementation agent due to its strong reductive ability. A set of reactions take place inside two cascaded reactors, and the chemical reactions are given as follows:

$$\mathrm{CuSO_4 + Zn \rightarrow ZnSO_4 + Cu\downarrow} \tag{1}$$
$$\mathrm{CuSO_4 + Cu + H_2O \rightarrow Cu_2O\downarrow + H_2SO_4} \tag{2}$$

The majority of copper ions react with zinc and precipitate as metallic copper. A portion of the deposited metallic copper further undergo comproportionation with ionic copper and form cuprous oxide precipitate.

In practice, the reactor is a typical continuously stirred tank reactor (CSTR). On the basis of the principle of material and mass balance, the dynamic model of CRP can be described by the following differential equations:

$$V\dot{C}_{\mathrm{Cu^{2+},1}} = QC^{\mathrm{in}}_{\mathrm{Cu^{2+},1}} - (Q+q)C_{\mathrm{Cu^{2+},1}} - Vr_{\mathrm{Cu^{2+},1}}, \tag{3}$$
$$\begin{aligned} V\dot{C}_{\mathrm{Cu^{2+},2}} &= (Q+q)C^{\mathrm{in}}_{\mathrm{Cu^{2+},2}} \\ &- (Q+q)C_{\mathrm{Cu^{2+},2}} - Vr_{\mathrm{Cu^{2+},2}}, \end{aligned} \tag{4}$$

where $C^{\mathrm{in}}_{\mathrm{Cu^{2+},i}}$, $i = 1, 2$ and $C_{\mathrm{Cu^{2+},i}}$, $i = 1, 2$ are the inlet and outlet concentrations of copper ions, respectively. $\dot{C}_{\mathrm{Cu^{2+},i}}$, $i = 1, 2$ is the respective change rate of copper ions concentration in ith reactor. V is the active volume of reactor. Q and q are the inlet solution flow rate and returned underflow rate. In particular, based on the kinetic modeling of the competitive-consecutive reaction, the sedimentation rate of copper ions of the ith reactor in CRP, $r_{\mathrm{Cu^{2+},i}}$, $i = 1, 2$, can be modeled by the following equations:

$$r_{\mathrm{Cu^{2+},1}} = (k_1 G_{\mathrm{Zn},1} + k_2)V^{-1}C_{\mathrm{Cu^{2+},1}}, \tag{5}$$
$$r_{\mathrm{Cu^{2+},2}} = (k_1 G_{\mathrm{Zn},2} + k_3)V^{-1}C_{\mathrm{Cu^{2+},2}}, \tag{6}$$

where $k_i, i = 1, 2, 3$ denotes kinetic parameters; $G_{\mathrm{Zn},i}$, $i = 1, 2$ denotes the zinc powder addition rate of the ith reactor.

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For the sake of simplicity, the dynamic model of the CRP can be rewritten as:

$$\dot{\boldsymbol{x}} = \boldsymbol{A}_1\boldsymbol{x} + \boldsymbol{A}_2\boldsymbol{x}^{\text{in}} + \boldsymbol{\phi}(\boldsymbol{x},\boldsymbol{u}) = \boldsymbol{F}(\boldsymbol{u}(t),\boldsymbol{x}(t),t), \tag{7}$$

$$\boldsymbol{A}_1 = \begin{bmatrix} -V^{-1}(Q+q) & 0 \\ 0 & -V^{-1}(Q+q) \end{bmatrix},$$
$$\boldsymbol{A}_2 = \begin{bmatrix} V^{-1}Q & 0 \\ 0 & V^{-1}(Q+q) \end{bmatrix},$$
$$\boldsymbol{\phi}(\boldsymbol{x},\boldsymbol{u}) = \begin{bmatrix} -V^{-1}(k_1u_1+k_2)x_1) \\ -V^{-1}(k_1u_1+k_3)x_2) \end{bmatrix},$$

where we denote zinc powder addition rate as control vector $\boldsymbol{u} = [G_{\text{Zn},1}, G_{\text{Zn},2}]$, the outlet copper ions concentration as state vector $\boldsymbol{x} = [C_{\text{Cu}^{2+},1}, C_{\text{Cu}^{2+},2}]$ and the inlet copper ions concentration as $\boldsymbol{x}^{\text{in}} = [C^{\text{in}}_{\text{Cu}^{2+},1}, C^{\text{in}}_{\text{Cu}^{2+},2}]$. Note that, the inlet reactant concentration of the #2 reactor is the outlet reactant concentration of the #1 reactor, namely $C^{\text{in}}_{\text{Cu}^{2+},2} = C_{\text{Cu}^{2+},1}$.

B. Production Constraints

1) Input constraints: The addition rates of zinc powder are the input variables of dynamic system in CRP. Here, we consider the input constraints which imposed by actuator limitations:

$$u_i^{\min} \le G_{\text{Zn,i}} = u_i(t) \le u_i^{\max}, i = 1,2, \tag{8}$$

where $u_i^{\min}$ and $u_i^{\max}$ are the allowed minimum and maximum rate of zinc powder to be added to the ith reactor.

2) Production constraints: For facilitating further downstream processing, outlet copper ion concentration of CRP needs to be reduced to a certain range precisely. Therefore, the state constraint of outlet copper ion concentration of #2 reactor $C_{\text{Cu}^{2+},2}$ must be satisfied as follow:

$$C^{\min} \le C_{\text{Cu}^{2+},2} = x_2(t) \le C^{\max}, \tag{9}$$

where $C^{\min}$ and $C^{\max}$ are the lower and upper bound.

3) Stability constraints: In copper removal process, the separation of copper is carried out with two cascaded reactors gradually. Most of copper ions are precipitated in the first reactor, and the second reactor serves as auxiliary for fine tuning. For better operation and stable production, copper removal rate $R_{\text{Cu}^{2+},1}$ of the #1 reactor (main reactor) should also meet the following constraint:

$$R^{\min} \le R_{\text{Cu}^{2+},1} = \frac{x_1^{\text{in}} - x_1(t)}{x_1^{\text{in}}} \le R^{\max}. \tag{10}$$

where $R^{\min}$ and $R^{\max}$ are the lower and upper bound, x_1^{in} denotes the inlet copper ions concentration of #1 reactor, so as to avoid the phenomenon of overreaction or insufficient reaction in the main reactor.

After three months of process observation and data collection, the process characteristic of the copper removal process can be shown in Table I.

TABLE I: Operating conditions for CRP (over 90 days)

Parameter	Unit	Value
Flow rate of leaching $ZnSO_4$ solution, Q	m^3/h	150-250
Flow rate of underflow, q	m^3/h	10-22
Solution volume, V	m^3	98-102
Inlet copper ion concentration, x_1^{in}	g/L	1.1-2.1
Desired outlet copper ion concentration, x_2	g/L	0.2-0.4

C. Dynamic Optimization Problem of CRP

After process analysis and modeling, a dynamic optimization problem of copper removal process can be described. The objective is to minimize the zinc addition consumption during the given time. The control variables are the feed rates of zinc addition in two stirred reactors. Since the reactions aim to precipitate the impurity copper, state variable path constraints must be imposed on the outlet copper ion concentration to keep it within a certain range throughout the entire process. Moreover, for better operation and stable production, the percentage of the removed copper of the main reactor should also meet the path constraint.

In summary, the dynamic optimization problem with continuous inequality constraints of CRP can be formulated as follow:

$$\min_{\boldsymbol{u}(t)} \quad J(\boldsymbol{u}(t)) = \int_{t_0}^{t_f} (u_1(t) + u_2(t))dt, \tag{11a}$$
$$\text{s.t. } \dot{\boldsymbol{x}} = \boldsymbol{F}(\boldsymbol{u}(t),\boldsymbol{x}(t),t) \tag{11b}$$
$$\boldsymbol{x}(t_0) = [x_1(t_0), x_2(t_0)] \tag{11c}$$
$$x_2(t) - C^{\max} \le 0 \tag{11d}$$
$$C^{\min} - x_2(t) \le 0 \tag{11e}$$
$$(x_1^{\text{in}} - x_1(t)) - R^{\max} \cdot x_1^{\text{in}} \le 0 \tag{11f}$$
$$R^{\min} \cdot x_1^{\text{in}} - (x_1^{\text{in}} - x_1(t)) \le 0 \tag{11g}$$
$$u_i^{\min} \le u_i(t) \le u_i^{\max}, i = 1,2 \tag{11h}$$
$$t \in [t_0, t_f], \tag{11i}$$

where $\boldsymbol{F}$ is the differential algebraic equation (DAE) constraint (7), describing the nonlinear dynamic process, $\boldsymbol{u}(t)$ denotes the control variable and $\boldsymbol{x}(t)$ is the state variable, $\boldsymbol{x}(t_0)$ is the initial state of the dynamic system at time t_0, and t_f is the final time, the objective function (11a) denotes the zinc addition consumption. The inequality path constraints (11d), (11e), (11f) and (11g), namely production constraints (9) and (10), can be unified as follow:

$$\boldsymbol{g}_i(\boldsymbol{x}(t)) \le 0, i = 1,2,3,4. \tag{12}$$

The optimization problem of CRP is a typical DOP with high nonlinearity, multidimensional, multimodal nature. Solving such kind of problem efficiently and accurately remains an issue, especially with the presence of constraints on both state and control. In the next section, a constrained dynamic optimization method is proposed to solve the DOPs with continuous inequality constraints.

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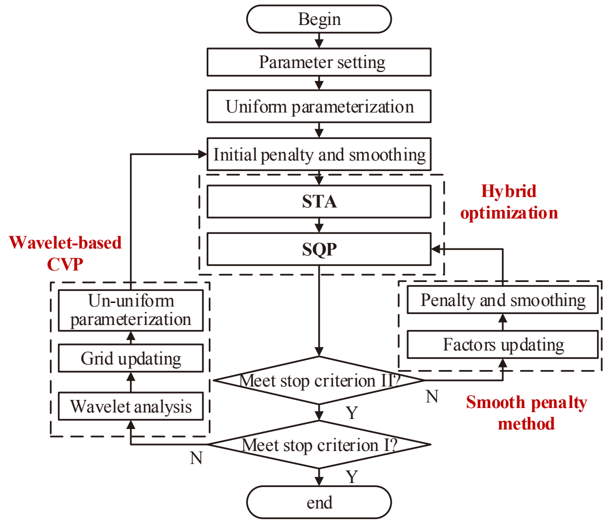

Fig. 3: Flow chart of the proposed method

III. Proposed Constrained Dynamic Optimization Method

The proposed constrained dynamic optimization approach consists of three essential parts. Firstly, a wavelet-based CVP method is investigated to reduce the original problem to a finite-dimensional NLP problem. Secondly, a smooth penalty function method is suggested to address the continuous equality constraints. Thirdly, a hybrid optimization strategy based on STA is proposed to solve the resulting unconstrained NLP problem robustly and efficiently. The whole framework of the proposed constrained dynamic optimization method is shown in Fig. 3.

A. Wavelet-based Control Vector Parameterization

With a prescribed parameterization scheme, usually an uniform piecewise-constant one, the original DOP can be approximated by a finite-dimensional NLP problem, and then solved by optimization algorithm. However, parameterizing the control variable uniformly always creates a serious flaw: a coarse resolution always leads to a poor approximation, while a fine resolution always brings over-parameterization, which puts a great challenge not only in the subsequent optimization but also in the implementation. Focus on above issues, a wavelet-based CVP suggested in [9] is adopted to generate an non-uniform parameterization scheme, which can assign appropriate resolution locally.

The wavelet-based CVP begins with a rough uniform parameterization scheme Ω_0. Applying this scheme, the control time horizon will be partitioned by a series of time knot $t_p, p = 0, ..., N$, where $N \geq 1$ is the number of the subintervals, with the knot points satisfying $t_0 < ... < t_p < ... < t_N = t_f$. Then, the control trajectory over the entire time span can be approximated as follows:

$$u(t) \approx \tilde{u}(t) = \sum_{p=1}^{N} \delta_p(t)\xi_p, t \in [t_0, t_f],$$

$$\delta_p(t) = \begin{cases} 1, t \in [t_{p-1}, t_p] \\ 0 \ \ , else \end{cases} ,p = 0, ..., N,$$

where $[t_{p-1}, t_p]$ is the pth control subinterval and ξ_p is the constant control value defined on the pth subinterval. So far, an optimal parameter selection problem has been yield, where the control values $\boldsymbol{\xi} = [\xi_1, \xi_2, ..., \xi_N]$ are the decision variables for the optimization.

As the optimal solution $\boldsymbol{\xi}^*$ under coarse parameterization grid Ω_0 is obtained, a wavelet-based refinement of time grid turns on. During the refinement process, the control trajectory $\tilde{u}(t)$ denoted by $\boldsymbol{\xi}^*$ is treated as a signal varying with time. The wavelet coefficients $d_{j,k}$ of $\tilde{u}(t)$ can be obtained through the fast wavelet transformation [15] with Haar basis. Here, j denotes the scale which responds to the level of resolution, and k denotes the translation index. Note that, small coefficient, i.e. $|d_{j,k}| \leq \epsilon_d$, implies that it only leads to a small change in the approximated $\tilde{u}(t)$, and thus the grid point here can be deleted for the subsequent optimization. On the other hand, large wavelet coefficient, i.e. $|d_{j,k}| > \epsilon_d$, means that a grid point insertion should be carried out here on a higher scale to approximate the strong variation. Here, the threshold ϵ_d is a user-specified parameter depending on the range of control values.

The main idea of this refinement strategy is to insert and delete the control grid point iteratively, by performing wavelet analysis on the previous generation's optimal solution. An example is shown in Fig. 4 to illustrate the wavelet-based grid refinement process. It can be seen that the lth optimal solution $\boldsymbol{\xi}_l^*$ with a rough grid Ω_l is analyzed, the grid point with small wavelet coefficient has been delete (marked by red "$\times$"), and four grid point (marked by red "$+$") has been inserted in scale $j = 3$. Thus a refined grid Ω_{l+1} is obtained for $(l+1)$th generation optimization.

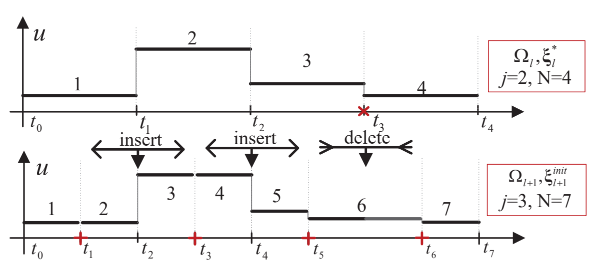

Fig. 4: Illustration of wavelet-based adaptive refinement

Based on the wavelet-based CVP method, the original DOP is approximated by a sequence of optimal parameter selection problems with continuous state inequality constraints. In next section, a smooth penalty method is adopted to handle the continuous constraints.

B. Smooth Penalty Method

The exact penalty function methods have been widely used for solving constrained optimization problems. After control parameterization, by appending the constraint violations to the cost function through a classic $l1$ penalty function, a modified cost function is yield:

$$J_1(\boldsymbol{\xi}) = J(\boldsymbol{\xi}) + \rho \int_{t_0}^{t_f} \sum_{i=1}^{m} \max\{\boldsymbol{g}_i(\boldsymbol{x}(t)), 0\}dt \qquad (13)$$

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where m is the number of the constraints, $\rho > 0$ is a penalty parameter, control values $\boldsymbol{\xi} = [\xi_1, \xi_2, ..., \xi_N]$ are the decision variables. However, it is noted that the penalty function max$\{\cdot,$ $0\}$ is not differentiable at boundary point x where $g_i(x) = 0$, which makes the gradient-based optimization struggle to handle. In order to address this issue, a smooth function [11] is introduced to approximate the non-smooth max penalty function:

$$S(y, \alpha) = \frac{1}{2}\left[\sqrt{y^2 + 4\alpha^2} + y\right] \tag{14}$$

where $y = g_i(\boldsymbol{x}(t))$, and α is a small positive number called smoothing parameter. The approximation property is shown in Fig. 5 and described as following formulas:

$$\lim_{\alpha \to 0^+} S(y, \alpha) = \max\{y, 0\}, \tag{15}$$

$$0 < S(y, \alpha) - \max\{y, 0\} \leq \alpha. \tag{16}$$

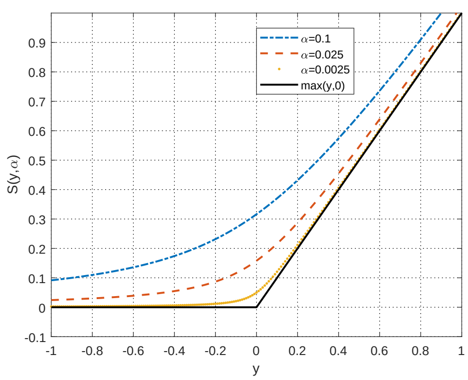

Fig. 5: The approximation property of $S(y, \alpha)$

From Fig. 5, it is obvious that there exists a width-varying gap between $S(y, \alpha)$ and $\max\{y, 0\}$, and the maximum difference occurs at $y = 0$, where constraint is active.

So far, an unconstrained smooth penalty problem has been yield as follow:

$$J_2(\boldsymbol{\xi}) = J(\boldsymbol{\xi}) + \rho \int_{t_0}^{t_f} \sum_{i=1}^{m} S\{g_i(\boldsymbol{x}(t)), \alpha)\} dt. \tag{17}$$

The smoothing factor α plays a critical role to adjust the approximation level. In order to obtain satisfied smoothing effect, the smoothing factor α needs to be large, while for pursuing an exact approximation, α should be set as small as possible. In other word, it facilitates the optimization at the expense of high approximate accuracy. In order to balance approximation accuracy and smoothness gradually, α is tend to be small and ρ is tend to be quite large as the iterations goes by. For sake of computational efficiency, α and ρ will be changed at the same time in next iteration optimization as $\alpha^* = d\alpha$ and $\rho^* = \rho/d$, where $0 < d < 1$ is a specified decrease factor. Note that minimizing smooth penalty problem (17) will force the constraint violation to be small enough as $\rho \to \infty$, and an approximate optimal solution of original constrained NLP problem can be obtained with sufficient accuracy as $\alpha \to 0$.

After parameterization and constraint handling, a sequence of unconstrained NLP problems are yield. In next section, a hybrid optimization strategy is proposed to solve above problems effectively and efficiently.

C. Hybrid Gradient State Transition Algorithm

1) Basic STA: STA is a global stochastic optimization algorithm, which has already exhibited excellent global search ability for solving various multimodal problems. Therefore, STA has potential advantages to solve above non-convex NLP problems. In STA, a solution to an optimization problem is considered as a state, and the update of solutions can be treated as state transition. As generation goes by, the solution will be transferred to the optimal state, by its special transformation operators, such as rotation, translation, expansion and axesion. A unified framework for state transformation can be described as follow:

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

where $\boldsymbol{x}_k \in \Re^n$ stands for an n-dimensional solution; $\boldsymbol{u}_k$ is a function of $\boldsymbol{x}_k$ and historical solutions; A_k and B_k are state transition matrices, which can denote different state transformation operators; $f(\cdot)$ is the fitness function, and y_{k+1} is the fitness of state $\boldsymbol{x}_{k+1}$.

2) HGSTA: Although STA has shown excellent global search performance, one of the interesting empirical observations we often observe is that the incremental improvement of such meta-heuristic optimization methods decreases rapidly as the iterations goes by. In the other words, a significantly increased computation can only bring minor improvements of objective function as current optima near the global optima. Meanwhile, it is known that gradient-based algorithms can find a local optima rapidly and accurately, owning to the utilization of gradient direction. Therefore, in order to accelerate the convergence speed in the local search phase, a hybrid optimization algorithm, named HGSTA, which combines STA and gradient-based method is proposed.

HGSTA is a hybrid optimization algorithm. In the first phase, STA is used to be responsible for the global search, aiming to provide a good starting point for next phase. The second phase is fine-tuning, a gradient-based method is adopted to enhance the local search ability. There are various gradient-based algorithms and here we use the sequential quadratic programming (SQP) method for its better behavior [16].

From Fig. 3, it is worth noting that, as the control grid has been fixed in each generation, STA solves the unconstrained NLP problem with initial smooth and penalty factors to locate the optimal solution roughly. Once a near-optimal solution has been obtained, a more accurate global optima can be found based on SQP and the iterative smoothing and penalty.

D. Proposed Constrained Dynamic Optimization Method Procedure

The pseudocode of the proposed constrained dynamic optimization method can be seen in Algorithm 1. It can be seen that solution accuracy can be improved by not only the iterative penalty function approximation process in the inner loop, but also the iterative grid refinement process in the outer loop. Therefore, the robustness, efficiency and precision can

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Algorithm 1 Pseudocode of the proposed constrained dynamic optimization method

```
Initialize refinement iteration l = 0, j = j_0, N = 2^{j_0};
Obtain the initial rough uniform parameterization gird Ω_0;
Initialize N-dimensional solution ξ_0 randomly;
while Stopping criterion I is not met do
    Set smooth penalty iteration n = 0, α = α_0, ρ = ρ_0;
    Transform constrained DOP to constrained NLP problem under gird Ω_l;
    Transform constrained NLP problem to unconstrained one (17) by smooth penalty function;
    Obtain the optimal solution of (17) by STA;
    while Stopping criterion II is not met do
        Obtain the optimal solution ξ_l^* of (17) by SQP;
        Let α = dα, ρ = ρ/d;
        Transform constrained NLP problem to unconstrained one (17) by smooth penalty function;
    end while
    Let l = l + 1, j = j + 1;
    Obtain the new grid Ω_l in scale j with ξ_{l-1}^*;
end while
```

be balanced by iteration. Note that all iterative optimization of refinement are warm-starting.

For stopping criterion I, it will be triggered by any of the following two conditions (18) and (19) which are formulated as follows:

$$\left|\frac{J_l - J_{l-1}}{J_{l-1}}\right| \le \varepsilon_s, \tag{18}$$

$$j > \overline{j}, \tag{19}$$

where ε_s is a stopping tolerance, l denotes the refinement iterations, $\overline{j}$ is the the maximum scale. Equation (18) denotes little relative improvement of J. It implies that a higher resolution of the control profile can not bring a corresponding improvement of approximation accuracy, and thus it's time to shut down the iterative refinement. The maximum scale $\overline{j}$ aims to limit the minimum operation time of each control value, because high-frequency control stemming from high solution will make it difficult and expensive to implement in practice.

For stopping criterion II, two conditions (20) and (21) have been taken into consideration, which are designed as follows:

$$\left|\frac{J_n - J_{n-1}}{J_{n-1}}\right| \le \varepsilon_s, \tag{20}$$

$$n > \overline{n}, \tag{21}$$

where n denotes the smooth penalty iterations, $\overline{n}$ is the maximum smooth penalty iteration. The little relative improvement of J between two iterations indicates that the smooth penalty function fits the original constrained optimization problem well. The maximum smooth penalty iteration $\overline{n}$ is designed to avoid sinking into the iterations for too long.

IV. Experiments and Discussion

In this section, in order to illustrate the efficiency of the proposed constrained dynamic optimization method, two cases of experiments are conducted: 1) a typical constrained DOP named Jacobson&Lele problem; and 2) the constrained DOP arising from CRP. All calculations are carried on MATLAB (Version R2017b) software platform using 3.4GHz Intel i7 PC with 8G RAM. Initial parameters, like α_0, ρ_0 and d are selected as 2.5×10^{-5}, 1 and 0.1. Termination parameters, like ε_s and $\overline{n}$ are set to 1×10^{-5} and 4. The initial and maximum scale are user-specified depending on problem. Parameter settings in STA can be found in [14].

A. Case I: Typical Industrial Problem

The Jacobson&Lele (J&L) problem is a typical industrial DOP proposed in [10]. This problem has a path state constraints, and its mathematics model can be described as follow:

$$\begin{aligned}
\min_{u(t)} \quad & J = x_3(t_f) \\
\text{s.t.} \quad & \dot{x}_1 = x_2 \\
& \dot{x}_2 = x_2 + u \\
& \dot{x}_3 = x_1^2 + x_2^2 + 0.005u^2 \\
& x_1 - 8(t-0.5)^2 + 0.5 \le 0 \\
& \boldsymbol{x}(0) = [0, -1, 0]^T \\
& -4 \le u \le 15 \\
& t_0 = 0, t_f = 1
\end{aligned}$$

The computational statistics for each generations is shown in Table II, where l denotes refinement iteration, j denotes scale, N denotes subinterval number, and $G = \sum_{i=0}^{m} \max\{g_i, 0\}$. The initial number j_0 and maximum scale number $\overline{j}$ are selected as 3 and 6.

During the test, the control variable is first discretized into 8 equidistant intervals. After 4 refinement, the solution is successively refined. Singular arcs is approximated with higher solution and flatness is merged, so that a desired approximation quality can be obtained with less discretization parameters. Besides, there is no violation of the path constraints because the $G = 0$ at the end of each inner penalty generation.

TABLE II: Iterative refinement process of the proposed constrained dynamic optimization method

Problem	l	j	N	ρ	α	G	J
J&L (min)	1	3	8	1	2.5e-4	0.0003	0.7445
				10	2.5e-5	0	0.7449
				100	2.5e-6	0	0.7449
	2	4	12	1	2.5e-4	0.00005	0.7389
				10	2.5e-5	0	0.7390
	3	5	17	1	2.5e-4	0	0.7383
				10	2.5e-5	0	0.7383
	4	6	26	1	2.5e-4	0	0.7381
				10	2.5e-5	0	0.7381

Comparison results is shown in Table III. First, it can be seen that the optimization results of HGSTA is better than STA, which denotes hybrid optimization has better local optimization ability. Second, the result from the proposed method

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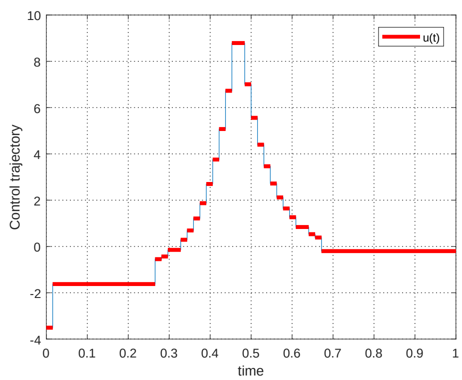
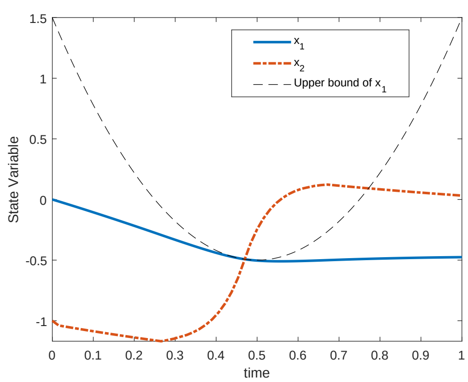
is in agreement with the results from the previous literatures, which verifies the validity of the results. Our result 0.7384 is better than 0.7485 obtained by improved CVP (ICVP) in [17], and much better than 0.79 obtained by orthogonal collocation (OC) in [18]. We can use only 26 control subintervals to obtain a satisfactory solution accuracy. The optimal control trajectory and state profiles of this problem obtained by proposed approach is illustrated in Fig. 6. From Fig. 6(b), it can be seen that x_1 is below its upper bound all along, which denotes the satisfaction of the path state constraint.

TABLE III: Comparison results of Case I

Problem	Method	Algorithm	J
J&L (min)	Proposed method	HGSTA	0.7381
		STA	0.7386
	ICVP [17]	-	0.7485
	GGM [18]	-	0.79



(a) Optimal control trajectory



(b) Optimal state profiles

Fig. 6: Optimal results of Case I

B. Case II: Industrial Experiment of CRP

Here, the proposed constrained dynamic optimization method is applied to solve the DOP (11) arising in CRP, so that an optimal operation trajectory of zinc powder addition can be obtained to precipitate copper ions into desirable concentration range with less zinc consumption. Three-month-long industry data of actual CRP was collected so as to verify the proposed approach's efficiency and robustness.

CRP is a part of the long process industry of zinc hydrometallurgy The inlet or outlet copper ion concentration can only be measured every 2 hours in the actual CRP, which is the key indicator of the working condition. In addition, according to the observation, the solution volume V and solution flow rates Q and q, have no obvious fluctuation in 2 hours. Therefore, we take 2 hours as the optimization interval, namely $t_0 = 0$ and $t_f = 2$, where V, Q and q remain constant. The dynamic optimization of CRP can be scheduled for every two hours, or if there is a significant discrepancy, new dynamic optimization results will be recomputed based on the current working conditions and used for the next 2 hours.

A dynamic optimization of 2 hours is carried out and the working condition in t_0 is shown in Table IV. Note that, the #2 outlet copper ion concentration $C_{\mathrm{Cu}^{2+},2}$ is the key variable which should be controlled in 0.2-0.4 g/L rigorously. Since a critical operation is unreliable in industrial practice under uncertainty, a back-off of 0.05 is highly desirable, such that $C_{\mathrm{Cu}^{2+},2}$ is subject to 0.25-0.35 g/L in this optimization.

TABLE IV: Operating conditions for CRP (over 2 hours)

Parameter	Unit	Value
Flow rate of leaching $ZnSO_4$ solution Q	m^3/h	200
Flow rate of underflow q	m^3/h	20
Solution volume V	m^3	100
Inlet copper ion concentration x_1^{in}	g/L	1.7
Initial #1 outlet copper ion concentration $\boldsymbol{x}_1(t_0)$	g/L	0.7
Initial #2 outlet copper ion concentration $\boldsymbol{x}_2(t_0)$	g/L	0.32
Zinc powder addition rate, u_i	kg/h	0-500
Copper removal rate of #1 reactor, $R_{\mathrm{Cu}^{2+},1}$	—	0.53-0.64

The computational statistics for each generations is shown in Table V, N_1 and N_2 are the subinterval number of u_1 and u_2. The initial number j_0 is selected as 2, and the maximum scale is set to 4 because each zinc powder addition rate should remain 7 minutes at least. During the test, the control variable is first discretized into 4 equidistant intervals. Faced with such a multi-variable dynamic optimization problem, control variables u_1 and u_2 are refined iteratively and respectively. The optimal control trajectory and state profiles of CRP obtained by proposed method are illustrated in Fig. 7.

Comparison results are shown in Table VI. We can see that the proposed method with HGSTA optimization has better local search performance than STA. The total zinc dust consumption of 2 hours under the optimal control is 463.8870 kg, which is much lower than the average amount of manual operation 510.37 kg. Thus, there exists a lot of waste of zinc powder in manual work in the actual industry. In addition, $G = 0$ in Table V and Fig. 7 both show that the outlet copper ion concentration meets the production constraints rigorously, which indicates the effectiveness of the proposed method.

V. Conclusion

In this work, dynamic optimization of CRP is conducted to find a time-varying zinc addition trajectory such that a desired outlet copper ion quality is achieved at the least

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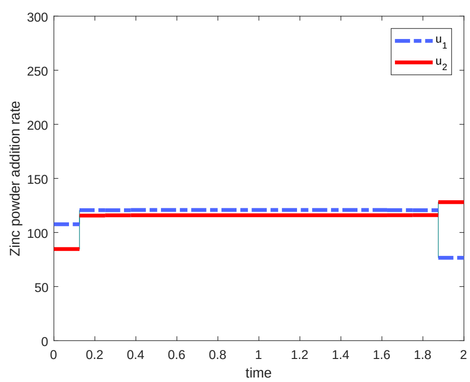
TABLE V: Iterative refinement process of the proposed constrained dynamic optimization method

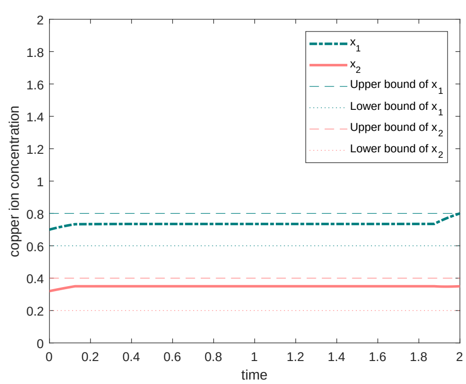
Problem	l	j	N_1	N_2	ρ	α	G	J
CRP (min)	1	2	4	4	1	2.5e-4	3.0783	429.2226
					10	2.5e-5	0.0023	468.2994
					100	2.5e-6	0	468.7325
					1000	2.5e-7	0	468.7323
	2	3	7	7	1	2.5e-4	0.6809	456.7708
					10	2.5e-5	0.0009	465.3369
					100	2.5e-6	0	465.4784
					1000	2.5e-7	0	465.4765
	3	4	7	7	1	2.5e-4	4.0543	413.6229
					10	2.5e-5	0.0002	463.8549
					100	2.5e-6	0	463.8888
					1000	2.5e-7	0	463.8870

TABLE VI: Comparison results of Case II

Problem	Method	Algorithm	J
CRP (min)	Proposed method	HGSTA	463.8870
		STA	465.3258
	Manual operation	-	510.3721



(a) Optimal control trajectory



(b) Optimal state profile

Fig. 7: Optimal results of Case II

zinc consumption for a given process time. After process analysis and modeling, a constrained DOP with one control constraints and two state constraints is constructed for CRP. A novel constrained dynamic optimization method is proposed to solve above DOP. First, the original infinite-dimensional problem is reduced to a finite-dimensional NLP problem based on wavelet-based CVP method which can generate an non-uniform parameterization grid adaptively. Second, a new smooth penalty function method is used to transform the constrained NLP problem into a sequence of unconstrained one. Third, a hybrid optimization strategy named HGSTA, which combines STA and gradient-based method, is proposed for solving the problem globally and efficiently. The simulation results show that the proposed method has good performance in solving constrained DOP, and the optimal zinc addition trajectory has promising applications in copper removal process.

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