Bi-objective Optimization of a Continuous Biological Process

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***Abstract*—This paper addresses the bi-objective optimization of continuous bio-dissimilation process of glycerol to 1, 3-propanediol. A bi-objective optimization model is firstly proposed to maximize the production rate of 1, 3-propanediol, simultaneously maximize the conversion rate of glycerol and ensure the bioprocess is operated under steady-state conditions. Then this bi-objective problem can be transformed into a sequence of single objective problems by using the weighted-sum and normal-boundary intersection methods respectively. Finally, these single objective problems are solved by an interior point method. The results show that the weighted-sum and normal-boundary intersection methods can obtain the approximate Pareto-optimal set of the proposed bi-objective optimization problem.**

Keywords-bi-objective optimization; weighted-sum method; normal-boundary intersection method; interior point algorithm; bio-dissimilation process

I. INTRODUCTION

1, 3-propanediol (1, 3-PD) has a wide range of potential applications on a large commercial scale [1]. Among all kinds of microbial production of 1, 3-PD, bio-dissimilation of glycerol to 1, 3-PD has been studied extensively since 1980s due to its relatively high yield and productivity [2]. In recent years, significant efforts from biochemical mechanism analysis, mathematical modeling, process optimization and robust control have been made to improve the dissimilation process of glycerol [2-10]. For example, research on the quantitative description of the cell growth kinetics of multiple-inhibitions, product formation in continuous culture has been made [3-5]. The nonlinear kinetic system of fed-batch fermentation was investigated in the process of glycerol bio-dissimilation to 1, 3-propanediol by *Klebsiella pneumoniae* [6]. A mathematical model was established to formulate the continuous culture of glycerol to 1, 3-propanediol by *Klebsiella pneumoniae* [7]. The optimal conditions of batch and continuous glycerol fermentations by *Klebsiella pneumoniae* were investigated using the volumetric productivity of 1, 3-propanediol as an optimization target based on a mathematical model that considers the growth kinetics of multiple inhibitions and the metabolic overflow of substrate consumption and product formation [2]. A robust controller was designed by using the bilinear transformation and H_∞ mixed sensitivity method for bio-dissimilation process of glycerol to 1, 3-propanediol [8]. A μ robust control strategy for continuous bio-dissimilation process of glycerol to 1, 3-propanediol has been proposed [9]. But the multi-objective optimization to this process has not yet been addressed.

The aim of this paper is to address the bi-objective optimization of continuous bio-dissimilation process of glycerol to 1, 3-propanediol by simultaneously maximizing the production rate of 1, 3-propanediol and the conversion rate of glycerol.

II. BI-OBJECTIVE OPTIMIZATION PROBLEM OF CONTINUOUS BIO-DISSIMILATION PROCESS OF GLYCEROL

A. Continuous Bio-dissimilation Process of Glycerol

The material balance equations of continuous bio-dissimilation process of glycerol to 1, 3-propanediol are written as follows [2]:

$$\frac{\mathrm{d}X}{\mathrm{d}t} = (\mu - D)X \tag{1}$$

$$\frac{\mathrm{d}C_{\mathrm{S}}}{\mathrm{d}t} = D(C_{\mathrm{S0}} - C_{\mathrm{S}}) - q_{\mathrm{S}}X \tag{2}$$

$$\frac{\mathrm{d}C_{\mathrm{PD}}}{\mathrm{d}t} = q_{\mathrm{PD}}X - DC_{\mathrm{PD}} \tag{3}$$

$$\frac{\mathrm{d}C_{\mathrm{HAc}}}{\mathrm{d}t} = q_{\mathrm{HAc}}X - DC_{\mathrm{HAc}} \tag{4}$$

$$\frac{\mathrm{d}C_{\mathrm{EtOH}}}{\mathrm{d}t} = q_{\mathrm{EtOH}}X - DC_{\mathrm{EtOH}} \tag{5}$$

where X is the biomass, gl^{-1}; D is the dilution rate, h^{-1}; C_{S0} and C_{S} are the substrate concentration (glycerol) in feed and reactor, respectively, mmoll^{-1}; C_{PD}, C_{HAc} and C_{EtOH} are the concentrations of products 1, 3-propanediol, acetic acid and ethanol, respectively, mmoll^{-1}; t is the fermentation time, h; μ, q_{S}, q_{PD}, q_{HAc} and q_{EtOH} are the specific growth rate of cells, specific consumption rate of substrate, specific formation rate

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of products 1, 3-propanediol, acetic acid and ethanol, respectively, mmolg^{-1}h^{-1}, which can be expressed as:

$$\mu = \mu_m \frac{C_S}{K_S + C_S}\left(1-\frac{C_S}{C_S^*}\right)\left(1-\frac{C_{PD}}{C_{PD}^*}\right)\left(1-\frac{C_{HAc}}{C_{HAc}^*}\right)\left(1-\frac{C_{EtOH}}{C_{EtOH}^*}\right) \quad (6)$$

$$q_S = m_S + \frac{\mu}{Y_S^m} + \Delta q_S^m \frac{C_S}{C_S + K_S^*} \quad (7)$$

$$q_{PD} = m_{PD} + \mu Y_{PD}^m + \Delta q_{PD}^m \frac{C_S}{C_S + K_{PD}^*} \quad (8)$$

$$q_{HAc} = m_{HAc} + \mu Y_{HAc}^m + \Delta q_{HAc}^m \frac{C_S}{C_S + K_{HAc}^*} \quad (9)$$

$$q_{EtOH} = q_S\left(\frac{b_1}{c_1 + DC_S} + \frac{b_2}{c_2 + DC_S}\right) \quad (10)$$

For *Klebsiella pneunoniae* cultivated under anaerobic conditions at 37 °C and pH 7.0, the maximum specific growth rate μ_m and the saturation constant for glycerol present the values of 0.67 h^{-1} and 0.28 mmoll^{-1}, respectively. The critical concentrations denoted as C^* in glycerol, 1, 3-propanediol, acetic acid and ethanol are 2039, 939.5, 1026 and 360.9 mmoll^{-1}, respectively. In addition, the parameters b_1, b_2, c_1 and c_2 in (10) are 0.025, 5.18, 0.06 and 50.45 mmoll^{-1}h^{-1}, respectively, while the ones for (7), (8) and (9) are listed in Table 1.

TABLE I. PARAMETERS IN THE MODELS (7)-(9)

Substrate/products	m	Y^m	Δq^m	K^*
Glycerol	2.20	0.0082	28.58	11.43
1, 3-propanediol	–2.69	67.69	26.59	15.50
Acetic acid	–0.97	33.07	5.74	85.71

B. Optimization Problem Statement

In this work, we propose the following bi-objective optimization problem of continuous bio-dissimilation process of glycerol to 1, 3-propanediol:

$$\max \quad f_1 = DC_{PD} \quad (11)$$

$$\max \quad f_2 = \frac{C_{S0} - C_S}{C_{S0}} \quad (12)$$

subject to satisfying:

$$(\mu - D)X = 0 \quad (13)$$

$$D(C_{S0} - C_S) - q_S X = 0 \quad (14)$$

$$q_{PD}X - DC_{PD} = 0 \quad (15)$$

$$q_{HAc}X - DC_{HAc} = 0 \quad (16)$$

$$q_{EtOH}X - DC_{EtOH} = 0 \quad (17)$$

$$0.05 \le D \le 0.5 \quad (18)$$

$$0 \le C_{S0} \le 2000 \quad (19)$$

$$0.05 \le X \le 3 \quad (20)$$

$$0 \le C_S \le 2039 \quad (21)$$

$$0 \le C_{PD} \le 939.5 \quad (22)$$

$$0 \le C_{HAc} \le 1026 \quad (23)$$

$$0 \le C_{EtOH} \le 360.9 \quad (24)$$

where the objective function f_1 is the production rate of 1, 3-propanediol, and f_2 is the conversion rate of glycerol; constraints (13)-(17) are the steady-state conditions; equations (18)-(24) are the lower and upper bounds for the optimized variables D, C_{S0}, X, C_S, C_{PD}, C_{HAc} and C_{EtOH} respectively. This set of constraints defines the *feasible space*, while the set of all possible values of the objective functions constitutes the *objective space*. Obviously, problem (11)-(24) is a bi-objective nonlinear programming with complex constants.

In bi-objective optimization problem (11)-(24), there does not exist a feasible solution that maximizes the objective functions f_1 and f_2 simultaneously. Therefore, attention is paid to *Pareto optimal solutions*; that is, solutions that cannot be improved in any of the objectives without degrading at least one of the other objectives. The set of Pareto optimal outcomes is often called the *Pareto front*.

III. OPTIMIZATION METHODS

Many strategies including weighted-sum method [11], weighted min-max method [12], normal-boundary intersection method [13], normal constraint method [14], genetic algorithms [15-16], and teaching–learning-based optimization algorithm [17] have been proposed to solve a bi-objective optimization problem. In this section, we firstly use the weighted-sum and normal-boundary intersection methods, respectively, to transform the bi-objective optimization problem (11)-(24) into a sequence of single objective problems. Then we use an interior point algorithm to solve these single objective problems.

A. Weighted-sum Method

In this subsection, we apply the weighted-sum method to turn optimization problem (11)-(24) into the following formulation:

$$\min \quad f = w\bar{f}_1 + (1-w)\bar{f}_2 \quad (25)$$

subject to satisfying:

$$(\mu - D)X = 0 \quad (26)$$

$$D(C_{S0} - C_S) - q_S X = 0 \quad (27)$$

$$q_{PD}X - DC_{PD} = 0 \quad (28)$$

$$q_{HAc}X - DC_{HAc} = 0 \quad (29)$$

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$$q_{\mathrm{EtOH}}X - DC_{\mathrm{EtOH}} = 0 \quad (30)$$

$$0.05 \le D \le 0.5 \quad (31)$$

$$0 \le C_{\mathrm{S0}} \le 2000 \quad (32)$$

$$0.05 \le X \le 3 \quad (33)$$

$$0 \le C_{\mathrm{S}} \le 2039 \quad (34)$$

$$0 \le C_{\mathrm{PD}} \le 939.5 \quad (35)$$

$$0 \le C_{\mathrm{HAc}} \le 1026 \quad (36)$$

$$0 \le C_{\mathrm{EtOH}} \le 360.9 \quad (37)$$

where $w \in [0,1]$ is the weighting factor; the new objective functions $\bar{f}_1$ and $\bar{f}_2$ have the following representations:

$$\bar{f}_1 = \frac{f_1^*(x_1^*) - f_1}{f_1^*(x_1^*) - f_1^{\min}} \quad (38)$$

$$\bar{f}_2 = \frac{f_2^*(x_2^*) - f_2}{f_2^*(x_2^*) - f_2^{\min}} \quad (39)$$

In this expression, x_i^* ($i = 1,2$) denote the optimal solutions of objective functions f_i ($i = 1,2$) under constraints (13)-(24), respectively, and $f_i^{\min}$ ($i = 1,2$) can be written as:

$$f_1^{\min} = \min\{f_1(x_1^*), f_1(x_2^*)\}$$

$$f_2^{\min} = \min\{f_2(x_1^*), f_2(x_2^*)\}$$

B. Normal-boundary Intersection Method

In this subsection, we introduce the normal-boundary intersection method to deal with bi-objective problem (11)-(24). This approach essentially works by solving sequentially a set of single optimization problems, which are defined as:

$$\max \quad \gamma \quad (40)$$

subject to satisfying:

$$\Phi\beta + \gamma n = F \quad (41)$$

$$(\mu - D)X = 0 \quad (42)$$

$$D(C_{\mathrm{S0}} - C_{\mathrm{S}}) - q_{\mathrm{S}}X = 0 \quad (43)$$

$$q_{\mathrm{PD}}X - DC_{\mathrm{PD}} = 0 \quad (44)$$

$$q_{\mathrm{HAc}}X - DC_{\mathrm{HAc}} = 0 \quad (45)$$

$$q_{\mathrm{EtOH}}X - DC_{\mathrm{EtOH}} = 0 \quad (46)$$

$$0.05 \le D \le 0.5 \quad (47)$$

$$0 \le C_{\mathrm{S0}} \le 2000 \quad (48)$$

$$0.05 \le X \le 3 \quad (49)$$

$$0 \le C_{\mathrm{S}} \le 2039 \quad (50)$$

$$0 \le C_{\mathrm{PD}} \le 939.5 \quad (51)$$

$$0 \le C_{\mathrm{HAc}} \le 1026 \quad (52)$$

$$0 \le C_{\mathrm{EtOH}} \le 360.9 \quad (53)$$

where Φ is a 2×2 payoff matrix in which the *i*-th column is $(\bar{f}_1(x_i^*), \bar{f}_2(x_i^*))^{\mathrm{T}}$; β is a vector of weights such that $\beta_1 + \beta_2 = 1$ and $\beta_i \ge 0$ ($i = 1,2$); $\Phi\beta$ defines the set of points that are convex combinations of the individual minima; n is called a quasi-normal vector defined as $\Phi \cdot [-1 \quad -1]^{\mathrm{T}}$; F is a vector with $F = (\bar{f}_1, \bar{f}_2)^{\mathrm{T}}$. As β is systematically modified, the solution to problem (40)-(53) yields an even distribution of Pareto optimal points representing the complete Pareto set.

C. Single Objective Optimization Solver

We use an interior point method [18-20] to efficiently solve both nonlinear optimization problems (25)-(37) and (40)-(53). This approach replaces the nonlinear programs (25)-(37) and (40)-(53) by a sequence of barrier subproblems of the forms (54)-(74) and (75)-(96) respectively.

$$\min \quad f_\mu = f + \mu \sum_{i=1}^{14} \ln(s_i) \quad (54)$$

subject to satisfying:

$$(\mu - D)X = 0 \quad (55)$$

$$D(C_{\mathrm{S0}} - C_{\mathrm{S}}) - q_{\mathrm{S}}X = 0 \quad (56)$$

$$q_{\mathrm{PD}}X - DC_{\mathrm{PD}} = 0 \quad (57)$$

$$q_{\mathrm{HAc}}X - DC_{\mathrm{HAc}} = 0 \quad (58)$$

$$q_{\mathrm{EtOH}}X - DC_{\mathrm{EtOH}} = 0 \quad (59)$$

$$D + s_1 - 0.5 = 0 \quad (60)$$

$$D - s_2 - 0.05 = 0 \quad (61)$$

$$C_{\mathrm{S0}} + s_3 - 2000 = 0 \quad (62)$$

$$C_{\mathrm{S0}} - s_4 = 0 \quad (63)$$

$$X + s_5 - 3 = 0 \quad (64)$$

$$X - s_6 - 0.05 = 0 \quad (65)$$

$$C_{\mathrm{S}} + s_7 - 2039 = 0 \quad (66)$$

$$C_{\mathrm{S}} - s_8 = 0 \quad (67)$$

$$C_{\mathrm{PD}} + s_9 - 939.5 = 0 \quad (68)$$

$$C_{\mathrm{PD}} - s_{10} = 0 \quad (69)$$

$$C_{\mathrm{HAc}} + s_{11} - 1026 = 0 \quad (70)$$

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$$C_{\mathrm{HAc}} - s_{12} = 0 \tag{71}$$

$$C_{\mathrm{EtOH}} + s_{13} - 360.9 = 0 \tag{72}$$

$$C_{\mathrm{EtOH}} - s_{14} = 0 \tag{73}$$

$$s_i > 0,\ i = 1,2,\ldots,14 \tag{74}$$

where s_i are the slack variables, and $\mu > 0$ is the barrier parameter.

$$\min \quad f_\mu = -\gamma + \mu \sum_{i=1}^{14} \ln(s_i) \tag{75}$$

subject to satisfying:

$$\Phi\beta + \gamma n = F \tag{76}$$

$$(\mu - D)X = 0 \tag{77}$$

$$D(C_{\mathrm{S0}} - C_{\mathrm{S}}) - q_{\mathrm{S}}X = 0 \tag{78}$$

$$q_{\mathrm{PD}}X - DC_{\mathrm{PD}} = 0 \tag{79}$$

$$q_{\mathrm{HAc}}X - DC_{\mathrm{HAc}} = 0 \tag{80}$$

$$q_{\mathrm{EtOH}}X - DC_{\mathrm{EtOH}} = 0 \tag{81}$$

$$D + s_1 - 0.5 = 0 \tag{82}$$

$$D - s_2 - 0.05 = 0 \tag{83}$$

$$C_{\mathrm{S0}} + s_3 - 2000 = 0 \tag{84}$$

$$C_{\mathrm{S0}} - s_4 = 0 \tag{85}$$

$$X + s_5 - 3 = 0 \tag{86}$$

$$X - s_6 - 0.05 = 0 \tag{87}$$

$$C_{\mathrm{S}} + s_7 - 2039 = 0 \tag{88}$$

$$C_{\mathrm{S}} - s_8 = 0 \tag{89}$$

$$C_{\mathrm{PD}} + s_9 - 939.5 = 0 \tag{90}$$

$$C_{\mathrm{PD}} - s_{10} = 0 \tag{91}$$

$$C_{\mathrm{HAc}} + s_{11} - 1026 = 0 \tag{92}$$

$$C_{\mathrm{HAc}} - s_{12} = 0 \tag{93}$$

$$C_{\mathrm{EtOH}} + s_{13} - 360.9 = 0 \tag{94}$$

$$C_{\mathrm{EtOH}} - s_{14} = 0 \tag{95}$$

$$s_i > 0,\ i = 1,2,\ldots,14 \tag{96}$$

where s_i are the slack variables, and $\mu > 0$ is the barrier parameter.

Both approximate problems (54)-(74) and (75)-(96) are a sequence of equality constrained problems. These are easier to solve than the original inequality-constrained problems (25)-(37) and (40)-(53).

Now we present the following algorithm to solve optimization problems (25)-(37) and (40)-(53):

(1) Choose an initial barrier parameter $\mu^{(0)}$, an initial iterate $(D^{(0)}, C_{\mathrm{S0}}^{(0)}, X^{(0)}, C_{\mathrm{S}}^{(0)}, C_{\mathrm{PD}}^{(0)}, C_{\mathrm{HAc}}^{(0)}, C_{\mathrm{EtOH}}^{(0)}, s_1^{(0)}, s_2^{(0)}, \cdots, s_{14}^{(0)})$ and the required accuracy. Set iterative counter $k = 0$.

(2) At the k-th ($k \geq 1$) iteration of the algorithm, compute and approximate solution of the barrier problem (25)-(37) or (40)-(53) by using a technique of switching between a line search method that computes steps by factoring the primal-dual equations and a trust region method that uses a conjugate gradient iteration [20]. By default, the algorithm first attempts to take a direct factorization step. If it cannot, it attempts a trust region iteration that guarantees progress toward stationarity is invoked.

(3) If the barrier problem (25)-(37) or (40)-(53) is solved to the required accuracy, then stop; else set

$$\mu^{(k)} = \alpha\mu^{(k-1)} \quad (0 < \alpha < 1)$$

$$k = k + 1$$

and go to step (2).

IV. Optimization Results

Figures 1 and 2 illustrate the Pareto front of bi-objective optimization problem (11)-(24) by using the weighted-sum and normal-boundary intersection methods. It can be seen that the production rate of 1, 3-propanediol and conversion rate of glycerol can not simultaneously reach their ideal points. However, a higher production rate of 1, 3-propanediol can be obtained if the conversion rate of glycerol belongs to the interval [0.94, 0.98]. From Figures 1 and 2, it can be observed that only fewer Pareto solutions were obtained by the weighted-sum approach when the production rate of 1, 3-propanediol is smaller than 20 $\mathrm{mmoll^{-1}h^{-1}}$. This concludes that the normal-boundary intersection method can yield a better distribution of Pareto front than the weighted-sum approach.

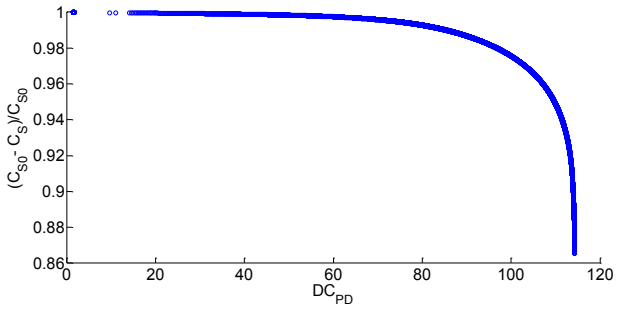

Figure 1. Pareto front with the weighted-sum method.

V. Conclusions

In this paper, we have addressed the bi-objective optimization of continuous bio-dissimilation process of

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glycerol to 1, 3-propanediol. The Pareto front of the proposed bi-objective model can be successfully obtained by using the weighted-sum and normal-boundary intersection methods. However, the normal-boundary intersection method obtains a better distribution of Pareto front than the weighted-sum approach. This suggests that the normal-boundary intersection method is a good choice for dealing with the bi-objective optimization of continuous bio-dissimilation process of glycerol to 1, 3-propanediol.

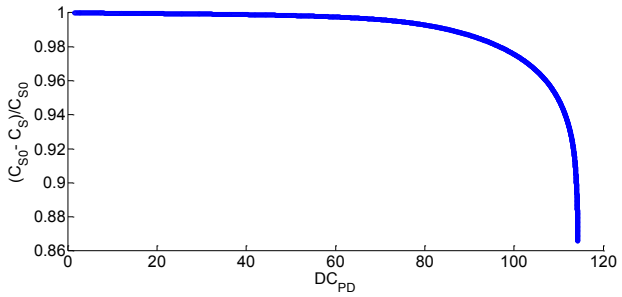

Figure 2. Pareto front with the normal-boundary intersection method.

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