Model predictive control of microbial fuel cell based on Kalman state estimation

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Abstract. Aiming at the constraints and undetectable interference in the microbial fuel cell system, a microbial fuel cell model predictive control method based on state estimation is proposed. According to the principles and actual requirements of the microbial fuel cell system, a state space model with input constraints is established. By introducing the model predictive controller, the performance of constrained optimization control is improved. Combined with the Kalman filter estimator, the impact of unmeasured interference on the predictive controller is compensated, and the control accuracy and robustness of the system are improved. The simulation experiment finally indicate that model predictive control based on kalman state estimation makes the output voltage of system reach the desired value, the input flow meets the actual demand and the cost is optimal. In addition, it has a good ability to deal with interference.

1. Introduction

The sustainable development of today's society is facing two major crises of energy shortage and environmental pollution [1]. The emergence of microbial fuel cell (MFC) provides a new way to solve these two crises. The use of microorganisms can convert the chemical energy of organic matter in sewage into electrical energy, which can achieve the purpose of purifying the environment and recovering energy [2-3]. At present, the research related to MFC system is still in the primary stage, and the problems such as low power density and unstable voltage lead to a certain gap from its practical application [4].

Many different methods have been proposed to improve the power generation performance of MFC by researchers, and most of the research mainly focuses on electrode materials, ion exchange membranes, and reactor structures. However, the research on MFC from the perspective of process optimization control is relatively less, Ravi et al. proposed an adaptive control method according to the characteristics of MFC in [5], the research shows that the adaptive compensation method can provide satisfactory results when the parameters are uncertain. Luo et al. proposed an improved feed-forward fuzzy logic PID algorithm in [6], research shows that the feed-forward fuzzy logic PID algorithm has better dynamic response and robustness than the traditional fuzzy PID when realizing the constant voltage control of the MFC system. Although these methods have certain effects in solving the uncertainty, nonlinearity, and interference of the MFC system, it is difficult to deal with constrained situations. The model
predictive control (MPC) does not require an accurate process model, and it has a good ability to deal with constraints [7]. An et al. proposed a MFC control based on a model predictive control strategy and achieved good control results in [8]. However, there are still limitations in the above research which does not consider the unmeasured interference in the actual industry. When these states cannot be fully measured, the MFC system will have low control accuracy and poor robustness. At the same time, it will cause frequent fluctuations in the production process, accelerate the loss of equipment, and affect the safe operation of the system.

Considering the input constraints and undetectable interference problems in the MFC system, a MFC model predictive control based on the state estimator is proposed in this paper to improve the ability of the system to operate safely and smoothly. The model predictive controller and state observer are designed based on MATLAB/Simulink platform. It can be seen from the simulation process that the proposed control method can effectively suppress the influence of unmeasurable disturbance, with high control accuracy and smoother control process. In addition, the system can maintain the ideal voltage output under different load disturbances and minimize the cost.

2. MFC mathematical model
MFC is mainly composed of anode, cathode, proton exchange membrane and electricity producing microorganism. In this paper, we mainly study MFC with acetate as the substrate, and establish the H-type two-compartment MFC mathematical model. The reaction process is as follows [9].

Anodic reaction

\[(\text{CH}_2\text{O})_2 + 2\text{H}_2\text{O} \rightarrow 2\text{CO}_2 + 8\text{H}^+ + 8e^- \quad (1)\]

Cathodic reaction

\[\text{O}_2 + 2\text{H}_2\text{O} + 4e^- \rightarrow 4\text{OH}^- \quad (2)\]

The expression of reaction rate in anode chamber is

\[r_1 = k_1^0 \exp \left( \frac{\alpha F}{RT} \eta_a \right) \frac{C_{AC}}{K_{AC} + C_{AC}} X \quad (3)\]

where \(C_{AC}\) and \(X\) are acetate and biomass concentrations, \(\eta_a\) represents anode overvoltage, \(k_1^0\) represents the anode reaction rate constant under standard condition (maximum growth rate ratio). \(K_{AC}\) represents the half rate constant of acetate, \(\alpha\) represents the charge transfer coefficient, \(F\) represents Faraday constant, \(R\) represents the gas constant, \(T\) represents the temperature of the MFC. The expression of reaction rate in cathode chamber is

\[r_2 = -k_2^0 \frac{C_{O_2}}{K_{O_2} + C_{O_2}} \exp \left( \frac{-(\beta - 1)F}{RT} \eta_c \right) \quad (4)\]

where \(C_{O_2}\) represents the concentration of dissolved oxygen, \(\eta_c\) represents the polarization overvoltage, \(K_{O_2}\) represents the half rate constant of dissolved oxygen, \(k_2^0\) represents the reaction rate constant of the cathode chamber under standard conditions, \(\beta\) represents the charge transfer coefficient.

We can regard the anode and cathode chamber of MFC as a dynamic equilibrium reaction process, so the four mass balance equations of the anode chamber can be obtained.

\[V_a \frac{dC_{AC}}{dt} = Q_a (C_{AC}^{in} - C_{AC}) - A_a r_1 \quad (5)\]

\[V_a \frac{dC_{CO_2}}{dt} = Q_a (C_{CO_2}^{in} - C_{CO_2}) + 2A_a r_1 \quad (6)\]

\[V_a \frac{dC_H}{dt} = Q_a (C_H^{in} - C_H) + 8A_a r_1 \quad (7)\]
\[
V_a \frac{dC_X}{dt} = Q_c \left( \frac{X^{in} - X}{f_X} \right) + A_m r_5 - V_a K_{dec} X
\]  
(8)

where the subscript \(a\) represents the anode, and the superscript \(in\) represents the feed, \(V\), \(Q\) and \(A_m\) represent the volume, flow rate and cross-sectional area of the film respectively. \(f_X\) is the reciprocal of the washed fraction, \(Y_w\) is bacterial yield, \(K_{dec}\) is the delay constant of using acetate. Similarly, the mass balance equation of the cathode chamber can be expressed by the following equation.

\[
V_c \frac{dC_{\alpha_1}}{dt} = Q_c (C_{\alpha_1}^{in} - C_{\alpha_1}) + A_m r_2
\]  
(9)

\[
V_c \frac{dC_{off}}{dt} = Q_c (C_{off}^{in} - C_{off}) - 4A_m r_2
\]  
(10)

\[
V_c \frac{dC_M}{dt} = Q_c (C_M^{in} - C_M) + A_m N_M
\]  
(11)

In the equation, the subscript \(c\) represents the cathode, \(N_M\) represents the flow of \(M^+\) through the proton exchange membrane from the anode to the cathode, which can be expressed as follows.

\[N_M = \frac{3600i_{cell}}{F}\]  
(12)

The charge balance equation are as follows.

\[C_a \frac{d\eta_a}{dt} = 3600i_{cell} - 8Fr_1\]  
(13)

\[C_c \frac{d\eta_c}{dt} = 3600i_{cell} + 4Fr_2\]  
(14)

where \(i_{cell}\) is current density, \(C_a\) and \(C_c\) are anode and cathode capacitors, respectively.

It is assumed that the ohmic loss at the wire connection point is ignored and that the internal resistance is caused by the resistance of the film and the solution. The total voltage of the MFC are as follows.

\[V_{cell} = V_0 - \eta_a + \frac{d_a}{k_a} + \frac{d_{cell}}{k_{aq}}i_{cell}\]  
(15)

where \(V_0\) is the open circuit voltage, \(d_a\), \(d_{cell}\), \(k_a\) and \(k_{aq}\) represent proton exchange film thickness, electrode spacing, film conductivity and solution conductivity, respectively.

Through the mathematical model of (3) ~ (15), the simulation model of system is established in MATLAB/Simulink and linearized, the steady-state point \((x_0, V_0)\) of anode model is \((2.25 \times 10^{-5}, -0.2274)\), and the steady-state point \((x_0, V_c)\) of cathode model is \((0.3 \times 10^{-5}, -0.5464)\).

The continuous state space equation of anode is as follows.

\[
A_e = \begin{bmatrix}
-0.4597 & -0.7976 & -0.3320 \\
0.0025 & -0.0019 & 0.0166 \\
-10.7391 & -169.3047 & -70.4708
\end{bmatrix}
B_e = \begin{bmatrix}
7545.5 \\
-369.2727 \\
-0
\end{bmatrix}
C_e = \begin{bmatrix}
0 & 0 & 1
\end{bmatrix}
\]  
(16)

The continuous state space equation of cathode is as follows.

\[
A_e = \begin{bmatrix}
-5.4760 & 4.3985 \\
1.8151 & -372.4917
\end{bmatrix}
B_e = \begin{bmatrix}
1132.7 \\
0
\end{bmatrix}
C_e = \begin{bmatrix}
0 & 1
\end{bmatrix}
\]  
(17)

The continuous state equation obtained above is discretized by approximate discretization.

\[x_a(k+1) = A_x x_a(k) + B_x u(k)\]  
(18)

\[y(k) = C_x x_a(k)\]
where $A_d = I + A_c T, \quad B_d = B_c T, \quad C_d = C_c$.

After the difference transformation, the incremental state space model is obtained.

$$
\begin{align*}
\dot{x}(k+1) &= Ax(k) + B_d u(k) \\
y(k) &= C\hat{x}(k)
\end{align*}
$$

(19)

where $A = \begin{bmatrix} A_d & O \\ C_d & A_d \end{bmatrix}, \quad B = \begin{bmatrix} B_d \\ C_d B_d \end{bmatrix}, \quad C = \begin{bmatrix} O & E \end{bmatrix}$. The Parameters are given in Table 1.

| Parameter  | Value                        | Parameter  | Value                        |
|------------|------------------------------|------------|------------------------------|
| $F$        | 96485.4 Coulombs mol⁻¹       | $V_a$      | $5.5 \times 10^{-5}$ m²      |
| $R$        | 8.3144 J mol⁻¹ K⁻¹          | $V_c$      | $5.5 \times 10^{-5}$ m²      |
| $T$        | 303 K                        | $A_m$      | $5 \times 10^{-4}$ m²        |
| $k_m$      | 17 Ohm⁻¹ m⁻¹                 | $f_k$      | 10                           |
| $d_m$      | $1.778 \times 10^{-4}$ m    | $C_{Ae}^{in}$ | 1.56 mol m⁻³          |
| $k_{aq}$   | 5 Ohm⁻¹ m⁻¹                  | $C_{O_2}^{in}$ | 0.3125 mol m⁻³          |
| $d_{cell}$ | $2.2 \times 10^{-2}$ m      | $U^0$      | 0.77 volt                    |
| $C_a$      | $4 \times 10^2$ F m⁻²       | $C_{M}^{i}_{C_{O_2}}, x_{i}^{in} , C_{H_i}^{in}, C_{OH}^{in}$ | 0 mol m⁻³       |
| $C_c$      | $5 \times 10^2$ F m⁻²       | /          | /                            |

3. MFC model predictive control based on state estimation

Considering the constraints and interference problems in MFC system, predictive control based on state estimation is used to optimize the whole MFC system. The control structure diagram of the whole algorithm in Figure 1. The state estimator obtains the optimal estimation of the state through the output and input of the system at the previous time, and the estimated state $\hat{x}(k)$ at the current time is input into the MPC controller, the prediction model takes $\hat{x}(k)$ as the initial state to predict the future dynamics of the system. At the same time, the optimal control sequence can be obtained by solving the constrained optimization problem, and only the first control sequence acts on the system.

![MFC model predictive control structure diagram based on state estimation](image)

Figure 1. MFC model predictive control structure diagram based on state estimation

3.1. Design of state estimator

The design of model predictive controller must know all the state information of the MFC, but in practice the state of the MFC cannot be fully measured, or interference and measurement noise exist. Kalman filter is an optimal state estimation method for the system with unmeasurable interference. The process of state estimation using Kalman filter recursive algorithm is as follows [10-11].

Discrete state model and measurement model:
\[ x(k + 1) = Ax(k) + B\Delta u(k) + w(k) \]  \hspace{1cm} (20)
\[ y(k) = Cx(k) + v(k) \]  \hspace{1cm} (21)

1) Calculate the state one-step prediction.
\[ \hat{x}(k | k - 1) = A\hat{x}(k - 1 | k - 1) + Bu(k - 1) \]  \hspace{1cm} (22)

2) Calculate the one-step prediction of estimation error covariance.
\[ P(k | k - 1) = AP(k - 1 | k - 1)A^T + Q \]  \hspace{1cm} (23)

3) Calculate Kalman gain.
\[ K(k) = P(k | k - 1)C^T (CP(k | k - 1)C^T + R(k))^{-1} \]  \hspace{1cm} (24)

4) Calculate the filter estimate value.
\[ \hat{x}(k | k) = \hat{x}(k | k - 1) + K(k)(y(k) - C\hat{x}(k | k - 1)) \]  \hspace{1cm} (25)

5) Update estimation error covariance.
\[ P(k | k) = (I - K(k)C)P(k | k - 1) \]  \hspace{1cm} (26)

where \( w(k) \) is the process input interference, \( v(k) \) is the measurement output interference, \( Q(k) \) and \( R(k) \) are noise covariance matrices.

3.2. Model predictive controller

The basic principle of MPC control consists of three steps [12-14]. Predicting the future dynamics of the system, solving the optimization problem and obtaining the control output; then rolling the time domain and repeating the above steps. The system state estimation \( \hat{x}(k) \) is obtained by Kalman filter, and the future state can be predicted according to the equation (19).

\[ \hat{x}(k + 1 | k) = Ax(k) + B\Delta \hat{u}(k | k) \]
\[ \hat{x}(k + 2 | k) = A\hat{x}(k + 1 | k) + B\Delta \hat{u}(k + 1 | k) \]
\[ \vdots \]
\[ \hat{x}(k + N_p | k) = A^{N_p}x(k) + BA^{N_p-1}\Delta \hat{u}(k | k) + A^{N_p-2}B\Delta \hat{u}(k + 1 | k) + \ldots + A^{N_p-N_c}\Delta \hat{u}(k + N_c - 1 | k) \]  \hspace{1cm} (27)

According to the predicted system state, the predicted output of the system can be obtained.

\[ \hat{y}(k + 1 | k) = CAx(k) + CBA\Delta \hat{u}(k | k) \]
\[ \hat{y}(k + 2 | k) = CA^2x(k) + CAB\Delta \hat{u}(k | k) + CBA\Delta \hat{u}(k + 1 | k) \]
\[ \vdots \]
\[ \hat{y}(k + N_p | k) = CA^{N_p}x(k) + CA^{N_p-1}B\Delta \hat{u}(k | k) + CA^{N_p-2}B\Delta \hat{u}(k + 1 | k) + \ldots + CA^{N_p-N_c}B\Delta \hat{u}(k + N_c - 1 | k) \]  \hspace{1cm} (28)

Define vector
\[ \hat{Y} = [\hat{y}(k + 1 | k) \ \hat{y}(k + 2 | k) \ \hat{y}(k + 3 | k) \ \ldots \ \hat{y}(k + N_p | k)]^T \]  \hspace{1cm} (29)
\[ \Delta \hat{U} = [\Delta \hat{u}(k | k) \ \Delta \hat{u}(k + 1 | k) \ \Delta \hat{u}(k + 2 | k) \ \ldots \ \Delta \hat{u}(k + N_c - 1 | k)]^T \]  \hspace{1cm} (30)

According to (28), (29) and (30), it can be concluded that
\[ \hat{Y} = F\hat{x}(k) + \Psi \Delta \hat{U} \]  \hspace{1cm} (31)

where
The optimization objective function can be described as

\[ J = \sum_{i=1}^{N_p} ||r(k+i|k) - y(k+i|k)||_2^2 + \sum_{i=0}^{N_r-4} ||\Delta u(k+i)||_2^2 \]  

(32)

where \( N_p \) is the prediction time domain and \( N_c \) is the control time domain. \( Q, R \) are weight matrices. In addition, the constraints of process operation variables must also be considered, anode/cathode control and incremental constraints can be described as

\[ u_{\text{min}} \leq u(k) \leq u_{\text{max}}, \quad \Delta u_{\text{min}} \leq \Delta u(k) \leq \Delta u_{\text{max}} \]  

(33)

(32) ~ (33) form a complete optimization objective expression. By transforming the optimization problem into a quadratic programming problem, the optimal control sequence can be obtained.

\[ \Delta \hat{U}^* = \left[ \Delta \hat{u}^*(k), \Delta \hat{u}^*(k+1), \ldots, \Delta \hat{u}^*(k + N_c - 1) \right]^T \]  

(34)

Only the first control sequence of the control increment sequence solved at each sampling time acts on the system, so its actual control input is

\[ u(k) = u(k-1) + \Delta \hat{u}^*(k) \]  

(35)

4. Simulation and analysis

In this paper, the MPC controller and state estimator of anode and cathode are designed. Firstly, the overvoltage of anode and cathode are controlled, and they are applied to the whole nonlinear MFC system. Finally, the output voltage of the whole MFC system is simulated. The anode MPC controller parameters \( N_C = 1, N_p = 9 \) and the cathode parameters \( N_C = 2, N_p = 10 \) in the simulation.

![Figure 2. Variation curve of anode control quantity](image_url)

![Figure 3. Variation curve of cathode control quantity](image_url)

The change curve of the anode and cathode control quantity are shown in Figure 2 and Figure 3. It can be seen from the figure that the anode and cathode feed flow can meet the actual input constraints under the action of the two controllers, but the control quantity curve under kalman-mpc is more gentle. With small fluctuation range and high steady-state accuracy. From the practical point of view, the use of kalman-mpc can better meet the economic indicators, it makes the feed flow value in an optimal state, and it will not significantly change up and down to damage the equipment, achieving the optimal cost.
In the simulation experiment, the curve of anode voltage variation and partial enlarged are shown in Figure 4 and Figure 5. It can be seen the kalman-mpc control method is 30% faster than the MPC control method in terms of amplitude. It can be seen from the partial enlarged diagram that the unmeasurable disturbance will affect the system, which makes the anode voltage in an unstable state. However, the kalman-mpc control method can effectively suppress the influence of disturbance, the control is more gentle and the steady-state accuracy is higher.

It is similar to the anode voltage experiment, the curves of cathode voltage variation and the partial enlarged diagram are shown in Figure 6 and Figure 7. It can be seen from the figure that noise disturbance will reduce the control performance of cathode MPC controller, and the MPC controller with Kalman correction can obtain stable cathode voltage output, which makes the control more smooth and steady-state precision higher, and effectively suppresses the influence of disturbance on the system.

The curve of anode voltage variation is shown in Figure 8. It can be seen from the diagram that the unmeasurable interference in the system will have a certain impact on the output of MFC system, and the control voltage will oscillate. The Kalman filter predictive control method proposed in this paper is more effective than the conventional feedback predictive control method to suppress the influence of unmeasured disturbance, the control process is more gentle, it has better robustness, and the steady-state accuracy is high.

In addition, the total voltage variation curve under load disturbance is shown in Figure 9. It can be seen from the figure that when the load suddenly changes at 90s and 160s, the constraint optimization
problem under the MPC controller has no feasible solution at 180s, so the simulation cannot continue, and the robustness is poor. The kalman-mpc control can keep the MFC system with ideal output and high steady-state accuracy. It shows that Kalman filter estimator has good anti-jamming ability and can improve the recursive feasibility of MPC controller.

5. Conclusion
Aiming at the problems of constraints and unmeasurable interference in the actual MFC system, a model predictive control based on state estimation is proposed. The simulation results show that the model predictive control using Kalman filter can make the system meet the actual constraints and work in the allowable operating range. At the same time, it effectively overcomes the influence of unmeasurable interference on the output of MFC system, improves the voltage tracking accuracy, has better stability, and significantly improves the control performance of the model predictive controller. In addition, when the load current changes suddenly, the model predictive control based on state estimation can quickly overcome the disturbance and make the system return to a stable state, which shows that it has good robustness.

Acknowledgments
This document is the results of the research project funded by the National Science Foundation of China granted No.61563032, No.61963025, the Open Foundation of the Key Laboratory of Gansu Advanced Control for Industrial Processes under Granted No.2019KX01, and The Project of Industrial support and guidance of Colleges and Universities in Gansu Province under Granted No.2019C-05.

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