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Model-based real-time optimisation of a fed-batch cyanobacterial hydrogen production process using economic model predictive control strategy

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HIGHLIGHTS

- On-line optimisation of fed-batch cyanobacterial hydrogen production process.
- Economic model predictive control formulation for process optimisation.
- Finite-data window least-squares procedure for model re-estimation.
- Hydrogen production increased by 28.7% compared to previous research.
- Model re-estimation frequency is essential for process on-line optimisation.

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ABSTRACT

Hydrogen produced by microorganisms has been considered as a potential solution for sustainable hydrogen production for the future. In the current study, an advanced real-time optimisation methodology is developed to maximise the productivity of a 21-day fed-batch cyanobacterial hydrogen production process, which to the best of our knowledge has not been addressed before. This methodology consists of an economic model predictive control formulation used to predict the future experimental performance and identify the future optimal control actions, and a finite-data window least-squares procedure to re-estimate model parameter values of the on-going process and ensure the high accuracy of the dynamic model. To explore the efficiency of the current optimisation methodology, effects of its essential factors including control position, prediction horizon length, estimation window length, model synchronising frequency, terminal region and terminal cost on hydrogen production have been analysed. Finally, by implementing the proposed optimisation strategy into the current computational fed-batch experiment, a significant increase of 28.7% on hydrogen productivity is achieved compared to the previous study.

1. Introduction

Hydrogen is considered as one of the fuels with great potential to provide clean energy for transport, electricity and heating in the future (Tamburic et al., 2011). At present, microorganisms such as green algae, cyanobacteria and purple non-sulphur bacteria have been extensively studied for biohydrogen production (Zhang et al., 2015c; Basak and Das, 2006). Many efforts have been conducted to identify biohydrogen synthesis metabolic mechanisms in different species (Melis et al., 2000; Min and Sherman, 2010; Bandyopadhyay et al., 2010; Zhang and Vassiliadis, 2015). Effects of culture composition, light intensity and temperature on biomass growth and hydrogen production have also been comprehensively explored from both simulation and experiment aspects (Basak and Das, 2006; Dechatiwongse et al., 2014; Oh, 2004; Zhang et al., 2015c, 2015b, 2015d, 2015e; Tamburic et al., 2012b) to determine the favourable conditions for biogas production. In addition, to facilitate the industrialisation of biohydrogen production process, a variety of novel photobioreactors (PBR) with different configurations have been designed to enhance hydrogen production and biomass density (Wang et al., 2013; Tamburic et al., 2011; Basak et al., 2014).

In order to accomplish the scale-up of hydrogen production from laboratory to industry, long term biogas production process has been conducted in recent studies. For example, a 21-day and a 23-day fed-batch process for green algal hydrogen production

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have been reported by Vijayaraghavan et al. (2009) and Kim et al. (2010), respectively. A 31-day continuous process for cyanobacterial hydrogen production has been carried out by Dechatiwongse et al. (2015). Similarly, a 24-day and a 30-day fed-batch process have also been developed by Lee et al. (2011) and Boran et al. (2010), respectively. Based on these studies, it is found that biogas productivity differs from 1.8 mL g^{-1} (biomass) h^{-1} to 37.9 mL g^{-1} (biomass) h^{-1} depending on both species nature and process operating conditions.

Despite these achievements, the low biogas productivity shown in recent studies still presents an open challenge for the industrialisation of biohydrogen production, and to fill this gap process optimisation becomes an indispensable tool to maximise the process performance. However, as hydrogen is only generated by green algae and cyanobacteria in anaerobic and nutrient-deprived cultures whilst cell growth happens in aerobic and nutrient-sufficient environments (Dechatiwongse et al., 2015), the incompatibility between biomass growth and biogas production conditions significantly complicates the optimisation of this process. As a result, although recent studies have tried to extend cell growth period and increase hydrogen production (Tamburic et al., 2012a, 2013), the results suggest that it is difficult to accurately estimate and control the addition of limiting nutrients during the entire process purely based on experiments. Therefore, to address this open challenge, a real-time dynamic optimisation framework has to be implemented.

Dynamic optimisation is the procedure of finding the optimal control by a given performance index (*e.g.* objective function) for a time-varying process. It has been extensively used for a number of off-line tasks in bioprocess simulation, including estimating parameter values for fermentation kinetic models (Zhang et al., 2015a; Adesanya et al., 2014), identifying desired operating conditions for batch and fed-batch processes (Del Río-Chanona et al., 2015; Alagesan et al., 2013), conducting operating studies in response to disturbances and upsets, and exploring the design of control systems (Biegler, 2014).

In spite of the wide application on off-line optimisation, it is notable that bioprocesses in general are networks of complex biochemical reactions manipulated by enzymes and affected by culture conditions, in which advanced regulation methods have to be carried out to ensure the performance and efficiency of the process. As a result, traditional off-line control may not be suitable for the optimisation of complicated bioprocess since small deviations between the on-going process and the expected behaviours can lead to significant losses in terms of process efficiency (Mailleret et al., 2004; del Rio-Chanona et al., 2015).

Model predictive control (MPC), on the other hand, is an on-line control implementation which is by now a well-established method for the optimal control of linear and non-linear systems (NMPC) (Grüne and Pannek, 2011). This method has become the most widespread advanced control methodology currently used in industry (Anon, 2013). The method approximates the solution of an infinite horizon optimal control problem, which is computationally intractable in general, by a sequence of finite horizon optimal control problems where the dynamic behaviour of the system is optimised over a prediction horizon by computing the optimal inputs over a control horizon (shown in Fig. 1). Then the first element of the resulting control sequence is implemented in each time step to generate a closed-loop static state feedback (Grüne and Pannek, 2009).

In particular, the Economic MPC (EMPC) approach is that in which an economic criterion (*e.g.* profitability, efficiency, production, etc.) is directly included in the performance index of the MPC formulation. This implementation achieves higher accuracy for process optimisation compared to the conventional MPC method, since it systematically determines the optimal operating strategy

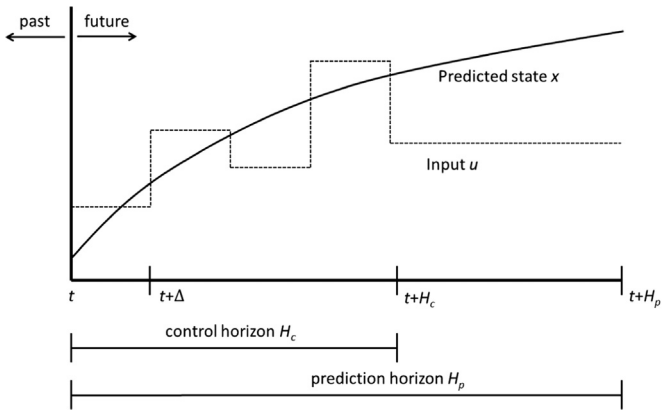

Fig. 1. Model predictive control framework.

Table 1
Parameters in the hydrogen production model.

Parameter	Value	Parameter	Value
$\mu_{max,h}$ h^{-1}	0.332	K_N mg	50.0
$\mu_{d,h}$ L h^{-1} g^{-1}	0.00716	$Y_{N/X}$ mg g^{-1}	492.7
k_q	0.165	$Y_{q/X}$ g^{-1}	0.0317
$k_{s,H2}$ μmol m^{-2} s^{-1}	140	$Y_{H/X}$ mL g^{-1} h^{-1}	14.20
$k_{i,H2}$ μmol m^{-2} s^{-1}	457	$Y_{O/X}$ L g^{-1}	81.02
Y_{Od} L g^{-2}	486.03	$Y_{C/X}$ mmol g^{-1}	20.454
Y_C mmol g^{-1} h^{-1}	0.0301	K_C mmol L^{-1}	0.0
α_g	0.0067	d_b m	0.002
k_s μmol m^{-2} s^{-1}	165	τ_c m^2 g^{-1}	0.126
k_i μmol m^{-2} s^{-1}	457	I_0 μmol m^{-2} s^{-1}	92.0
L m	0.025	T °C	35.0

based on the real time economic measurements whilst accounting for state constraints, input constraints and time-varying constraints (Biegler, 1998; Ellis and Christofides, 2013; Bemporad and Morari, 1999). Therefore, in the current study an EMPC strategy is employed to maximise biohydrogen production in a real-time framework by administering the optimal influent nutrient flow rate over the entire process.

2. Methodology theory

2.1. Dynamic model for cyanobacterial hydrogen production

In the current study, cyanobacterium *Cyanothece* sp. ATCC 51142 is selected due to its high hydrogen productivity (Bandyopadhyay et al., 2010). In our previous study (Zhang et al., 2015b, 2015d), a dynamic model has been proposed to simulate the entire batch process from cyanobacterial photo-heterotrophic growth to hydrogen production, and is shown in Eqs. (1a) to (1m). The detailed experimental setup and model construction can be found in Zhang et al. (2015b, 2015d). Parameter values in the model are listed in Table 1. When simulating a fixed volume fed-batch process where dense nitrate (0.5 mol L^{-1}) and glycerol (0.1 mol L^{-1}) solutions are fed into the reactor, Eqs. (1b) and (1f) are replaced by Eqs. (1n) and (1o).

$$\frac{dX}{dt} = \bar{k}(I)\bullet\mu_{max,h}\bullet\left(1-\frac{k_q}{q}\right)\bullet X\bullet\frac{C}{C+K_C}-\mu_{d,h}\bullet X^2 \tag{1a}$$

$$\frac{dN}{dt} = -Y_{N/X}\bullet\bar{k}(I)\bullet\mu_{max,h}\bullet\frac{N}{N+K_N}\bullet X \tag{1b}$$