Application of conventional nonlinear model predictive control (NMPC) and economic nonlinear model predictive control (E-NMPC) for technical and economical optimization of biochemical reactor system

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Application of Conventional Nonlinear Model Predictive Control (NMPC) and Economic Nonlinear Model Predictive Control (E-NMPC) for Technical and Economical Optimization of Biochemical Reactor System

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Abstract. This paper studies the application of Economic Nonlinear Model Predictive Control (ENMPC) and conventional NMPC to a biochemical reactor system with variation in reaction kinetics and disturbance values. The controlled variable for this study is the biomass concentration of the outlet stream leaving the reactor. To control it, conventional NMPC scheme which minimizes the controlled variable deviation to a desired set point and ENMPC scheme which optimizes the biomass production of the system are simulated against disturbance in reactor feed substrate concentration. Result shows that the conventional NMPC schemes are able to bring or maintain the controlled variable to a desired set point. However, the ENMPC scheme outperform the conventional NMPC in cumulative biomass production along the simulation period of up to 57% at the cost of higher computational time.

INTRODUCTION

Chemical products which are synthesized with processes based on biochemical reactions have seen significant increase in demand over the years. These products which include foods and beverages, pharmaceuticals, and several commodity and specialty chemicals are created with a series of reaction and separation or purifying processes. The reaction processes are usually based on cellular reaction, typically in the form of aerobic or anaerobic fermentation of a known substrate, which changes it to the desired chemicals with the help of microorganisms or enzymes. Advances in recombinant DNA technology have paved the way to an increase in yield for biochemical processes by means of improved genetically engineered cell strains [1].

Biochemical reactors used as the main equipment for the core process of biochemical products synthesis are usually operated either fed-batch or continuously. A fed-batch reactor stops the inlet and outlet flow as the reaction progresses, only letting the products flow out after a certain amount of time has passed. Meanwhile, a continuous biochemical reactor maintains the same flow rate of both substrate feed and product outlet of the reactor as to maintain a constant volume of matter inside the reactor. As for the type of reactors, one of the most commonly used for large scale synthesis is the stirred-tank bioreactor [2]. Bioreactors themselves present unique modeling and control challenges compared to conventional reactors owing to the complexity of the underlying biochemical reactions involved [3].

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As all other chemical processes, operating in a stable and economically optimal range is crucial. To achieve such condition for a complex system, especially those with strong nonlinearities such as biochemical reactors, an advanced control scheme is needed. One such control scheme is model predictive control (MPC). MPC is a control methodology that accounts for performance criterion by optimizing a cost function over a finite-time prediction horizon subject to a process model, process constraints, and stability constraints [4]. To address the system's nonlinearities along with an economical objective for the controller, a nonlinearized model of the system along with modification of the cost function of the MPC scheme are required, producing a control methodology known as economic NMPC. Economic NMPC itself is a modified NMPC which main different lies in the objective function which the controller maximizes or minimizes.

There have been several researches which applied economic MPC as a controller to optimize both linearized and nonlinearized systems such as boiler-turbine by Liu and Cui [5], solid sorbent-based CO_2 capture by Yu and Biegler [6], gas lifted well network by Suwartadi et al [7], absorber-stripper CO_2 capture process by Chan and Chen [8], and catalytic pyrolysis by Wang et al [9]. Several researches regarding conventional NMPC application have also been done, such as by Diehl et al [10] in oil production and Noga et al [11] in superfluid helium cryogenics. Another research by Mukhifullah uses a biochemical reactor system with an adaptive PID control scheme [12]. However, there have been no research which uses a biochemical reactor system as a basis for E-NMPC scheme. Therefore, in this paper, an evaluation of feasibility and performance of E-NMPC and NMPC, based on minimization of objective function based on SP deviation for NMPC and cumulative production for E-NMPC, applied to a biochemical reactor system will be done.

PROCESS DESCRIPTION AND PROBLEM DEFINITION

Biomass synthesis process with continuous stirred-tank reactor

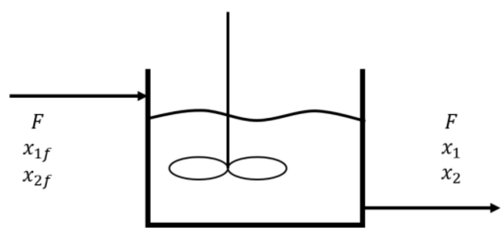

FIGURE 1. Biochemical reactor simplified process flow diagram

The process flow diagram of the system is shown in Figure 1. The system used is a continuous stirred-tank bioreactor with two components, substrate and biomass. An inlet stream of substrate with a flow rate of F and concentration of x_{2f} enters the reactor with a volume of V. The substrate mixes with the substrate that accumulates in the reactor and reacts. The reactor is assumed to be well-mixed and produces a solution with substrate concentration of x_2 and biomass concentration of x_1. The reaction is assumed to follow substrate inhibition kinetic model, which governs the reaction rate of both substrate and biomass through a value called growth rate coefficient μ. To maintain a constant reactor volume, the flow rate of the outlet stream is kept the same with the inlet flow rate F. Considering that the volume of reactor is kept constant and the inlet and outlet flow rate is the same, the flow rate could be represented in a term called dilution rate D, which is a ratio of the flow rate and the reactor volume. To model the relation of substrate consumption and biomass production kinetics, a term called yield Y is introduced, which is the ratio between the rate of biomass production r_1 and the rate of substrate consumption r_2. The outlet stream has the same composition with the solution in the reactor, that is a biomass concentration of x_1 and substrate concentration of x_2. The parameters for the system are taken from the model presented by Bequette [13].

The equations governing the dynamics of this system are as follows:

$$D = \frac{F}{V} \tag{1}$$

$$\mu = \frac{\mu_{\max} x_2}{k_m + x_2 + k_1 x_2^2} \tag{2}$$

$$r_1 = \mu x_1 \tag{3}$$

$$Y = \frac{r_1}{r_2} \tag{4}$$

$$\frac{dx_1}{dt} = (\mu - D)x_1 \tag{5}$$

$$\frac{dx_2}{dt} = D\left(x_{2f} - x_2\right) - \frac{\mu x_1}{Y} \tag{6}$$

Problem definition

Conventional controller that is currently used typically has a two layered hierarchy. The first layer computes the optimal steady state condition, which is transferred as a set point for the second layer, which is a reference tracking controller which bring process parameters to the desired set point. In this case, a single layered economic NMPC will be used which simultaneously calculate the optimal steady state and bring the process parameters to converge with said set point.

The system that is simulated is assumed to be an ideal system, where no unmeasured disturbance is present on the system and no noise is present on the transmitter of the controller. By these assumptions, state estimation could be simplified by assuming that the state estimated from the model represents the actual state of the system, that is, no plant-model mismatch is present for this case study. Thus, use of measurement filter such as the unscented kalman filter (UKF) or extended kalman filter (EKF) which are typically used for nonlinear systems with disturbance's state estimation is not necessary.

The controlled system is given by the following discrete-time nonlinear system:

$$\hat{x} = f(x, u) \tag{7}$$

$$y = h(x) \tag{8}$$

where $x \in \mathbb{R}^{n_x}$ is the current state, $\hat{x} \in \mathbb{R}^{n_x}$ is the estimated state based on current sate and current input, $u \in \mathbb{R}^{n_u}$ is the current input, and $y \in \mathbb{R}^{n_y}$ is the current output. The function $f(x, u)$ and $h(x)$ are assumed to be continuously differentiable. The modified cost function for the economic NMPC is based on maximization of biomass production as follows:

$$\max_{x,u} \sum_{i=0}^{P-1} g(y_i, u_i) \tag{9}$$

subject to:

$$x_0 = \hat{x} \tag{10}$$

$$x_{i+1} = f(x_i, u_i), \qquad y_i = h(x_i) \tag{11}$$

$$y_i \in \mathbb{Y}, \qquad u_i \in \mathbb{U} \tag{12}$$

Where P is the controller's prediction horizon, $x = (x_0, x_1, \ldots, x_P)$ are state sequence, and $u = (u_0, u_1, \ldots, u_P)$ are input sequence. $\mathbb{Y}$ and $\mathbb{U}$ are output and input constraints applied to the controller scheme. The function $g(y_i, u_i)$ represents the instantaneous biomass production of the system, represented by:

$$g(y_i, u_i) = X_1 . F \tag{13}$$

where X_1 is the reactor outlet stream's biomass concentration, and F is the flowrate of the stream leaving the reactor. For conventional NMPC algorithm, the function $g(y_i, u_i)$ is a tracking cost function which minimizes the state variables deviation from a defined set point.

For this study, the output is not constrained as it will follow the controller's decision variables. The input, which is the reactor's inlet and outlet flowrate (F) are constrained, where:

$$0.1 < F < 2 \tag{14}$$

The evaluation done in this study will be done for two types of reaction kinetics, which are monod and substrate inhibition model. The parameters used for the biochemical reactor system and controller are shown in Table 1 and Table 2.

TABLE 1. Parameters for monod and substrate inhibition model.

Monod	Substrate Inhibition
μ_{max} = 0.53 hr^{-1}	μ_{max} = 0.53 hr^{-1}
k_m = 0.12 g/liter	k_m = 0.12 g/liter
Y = 0.4	k_1 = 0.4545 liter/g
x_{2f} = 4.0 g/liter	Y = 0.4
	x_{2f} = 4.0 g/liter

TABLE 2. Controller tuning parameters

Disturbance (x_{2f})	ENMPC	NMPC, Single SP	NMPC, Changing SP
Monod +50%	T_s = 0.1 hr P = 18; M = 12	T_s = 0.1 hr P = 28; M = 9	T_s = 0.1 hr P = 21; M = 11
Monod -14%	T_s = 0.1 hr P = 20; M = 10	T_s = 0.1 hr P = 28; M = 5	T_s = 0.1 hr P = 25; M = 12
Substrate Inhibition +50%	T_s = 0.1 hr P = 28; M = 10	T_s = 0.1 hr P = 7; M = 7	T_s = 0.1 hr P = 28; M = 9
Substrate Inhibition -9%	T_s = 0.1 hr P = 16; M = 11	T_s = 0.1 hr P = 23; M = 5	T_s = 0.1 hr P = 23; M = 1

SIMULATION RESULTS

This section will present the result of simulating the system's controlled dynamic behaviour using ENMPC and conventional NMPC. The parameters used for these simulations are provided in Table 1 and Table 2. Positive and negative step disturbances are given to the feed substrate composition at the 101st iteration. This disturbance is used to simulate known changes in feed composition for causes such as procurement issues. All simulations presented are done in MATLAB R2019a.

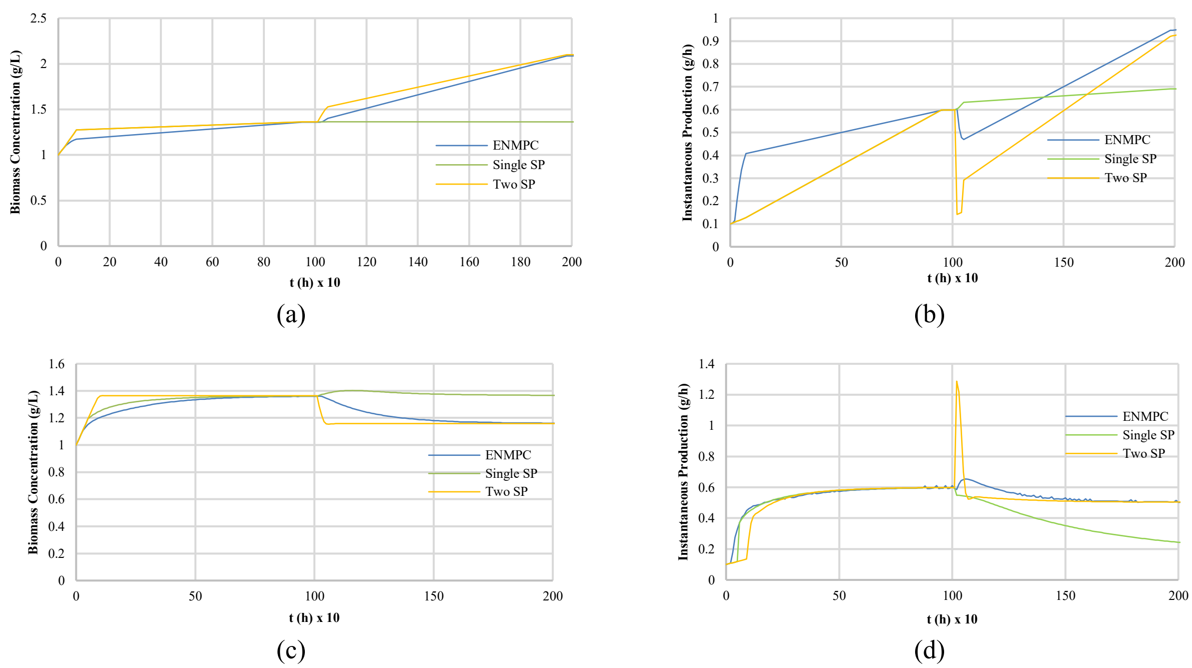

FIGURE 2. Controlled system dynamic concentration profile to +50% (a) and -14% (c) disturbance of x_{2f} and their respective instantaneous production dynamic profile (b,d) for monod kinetics

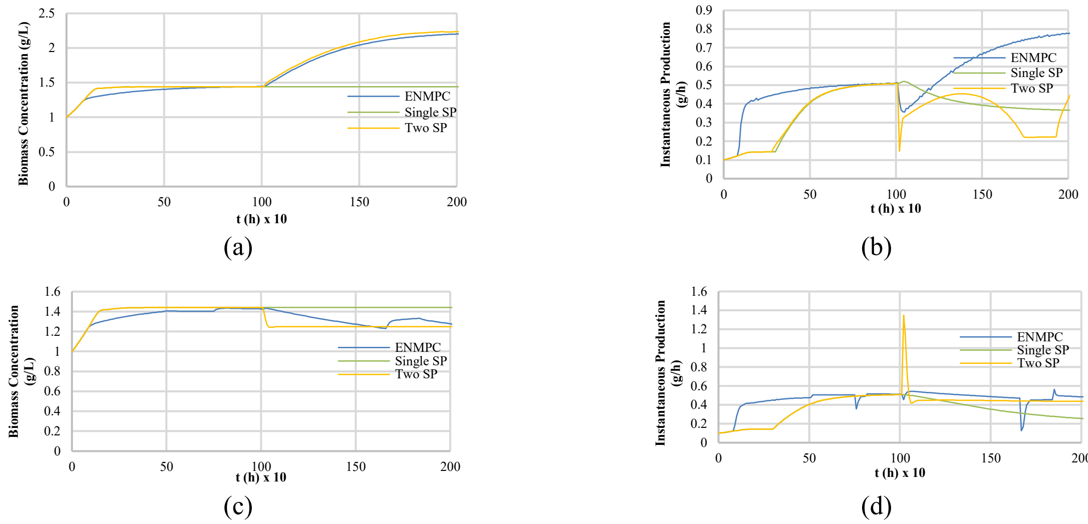

FIGURE 3. Controlled system dynamic concentration profile to +50% (a) and -9% (c) disturbance of x_{2f} and their respective instantaneous production dynamic profile (b,d) for substrate inhibition kinetics

TABLE 3. Cumulative biomass production

Disturbance (x_{2f})	ENMPC	NMPC, Single SP	NMPC, Changing SP
Monod +50%	13.35 g	12.05 g	10.36 g
Monod -14%	10.87 g	9.12 g	10.60 g
Substrate Inhibition +50%	10.74 g	7.54 g	6.83 g
Substrate Inhibition -9%	9.32 g	7.09 g	8.07 g

TABLE 4. Computation time

Disturbance (x_{2f})	ENMPC	NMPC, Single SP	NMPC, Changing SP
Monod +50%	2335.41 s	51.03 s	88.12 s
Monod -14%	1820.03 s	16.23 s	26.45 s
Substrate Inhibition +50%	1011.10 s	61.31 s	154.23 s
Substrate Inhibition -9%	3097.61 s	48.41 s	39.09 s

The dynamic response of the system against positive and negative disturbances are shown in Figure 2 and Figure 3. The controlled variable process reaction curve shows that the conventional NMPC schemes are able to bring the biomass concentration to a desired value. The ENMPC scheme, however, naturally changes the biomass concentration to optimize its production in the system. From t = 0 to t = 10 h, we could see that the NMPC schemes are faster at achieving the desired set point while the ENMPC, although lags behind, has higher biomass production. This could be understood as to increase the biomass concentration in the reactor, the controller has to increase the residence time of the reactant by lowering the dilution rate. This lowering of dilution rate, however, causes the biomass production to be hindered considering that the biomass production is proportional to the system's dilution rate. Therefore, it could be seen that the ENMPC scheme optimize the transient behaviour of the system.

At t =10 h, disturbance is introduced to the system and the controllers will give the best response to achieve their objective function. For the conventional NMPC scheme, this objective function penalizes the controlled variable's deviation against the desired set point. The conventional NMPC schemes are able to bring the controlled variable value to a desired set point despite the process disturbance. Similar behaviours are observed from the onset of disturbance, where the single SP NMPC shows almost no changes in the biomass concentration, indicating a good control performance, while the changing SP NMPC shows a sharper change than the ENMPC scheme. For the positive disturbance, the biomass production of the single SP NMPC is outperformed by the ENMPC due to its requirements to maintain the biomass concentration despite the higher substrate feed, which is achieved by lowering the system's dilution rate at the expense of its production rate. The changing SP NMPC is outperformed by the same reason as the simulation from $t = 0$ to $t = 10$ h, where the ENMPC is better at transient optimization of the system. Overall, the ENMPC are better at optimization of biomass production than the conventional NMPC schemes as shown in Table 3. This increased production, however, comes at a cost of higher computation power, as the ENMPC not only has to optimize the dynamic behaviour of the controlled variable, but also for this case, the interaction of the controlled variable with the dilution rate.

CONCLUSIONS

Application of ENMPC and conventional NMPC for a continuous stirred-tank biochemical reactor system are studied in this work. Conventional NMPC has the ability to maintain or bring the biomass concentration to a desired set point value despite large disturbance in feed substrate composition. The ENMPC controller which is intended to optimize biomass production is able to outperform both case of conventional NMPC in biomass production of up to 57% at the cost of significantly higher computation time. This optimization is rooted in the transient dynamics which is optimized in ENMPC but not in conventional NMPC.

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