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An Integrated Biomimetic Control Strategy with Multi-agent Optimization for Nonlinear Chemical Processes ⋆

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Abstract: In this paper, a framework is proposed for integrating a Biologically-Inspired Optimal Control Strategy (BIO-CS) with Multi-Agent Optimization (MAO) algorithms for process systems engineering applications. In this framework, the BIO-CS employs gradient-based optimal control solvers in an intelligent manner to simultaneously control multiple outputs of the process at their desired setpoints. Also, the MAO uses the capabilities of nonlinear heuristic-based optimization techniques such as Efficient Ant Colony Optimization (EACO), Efficient Genetic Algorithm (EGA) and Efficient Simulated Annealing (ESA) by sharing process information to obtain as an upper layer optimal operating setpoints for the controller that satisfy the overall process objective. The resulting approach is a unique combination of control and optimization methods that provide optimal solutions for dynamic systems. The applicability of the proposed framework is demonstrated using a nonlinear, multivariable fermentation process. In particular, a multivariable control structure associated with the first-principles-based model derived from mass and energy balances of the fermentation process is addressed. The performance of the proposed approach for each step is compared to Sequential Quadratic Programming (SQP) and a classical Proportional-Integral (PI) controller in terms of optimization and control, respectively. The proposed approach improves the overall performance of the process in terms of cumulative production rate by approximately 10-15%, resulting in economic benefits. The obtained results illustrate the capabilities of this novel integrated framework to achieve desired nonlinear system performance considering scenarios associated with setpoint tracking and plant-model mismatch.

Keywords: Nonlinear Control, Optimal Control, Agents, Optimization, Intelligent Control

1. INTRODUCTION

Biomimetic methods are the human-made designs that mimic biological systems. This area has gained a lot of attention in recent years from researchers in various disciplines. These methods are also emerging in chemical engineering applications, including process systems engineering. For example, a Biologically-Inspired Optimal Control Strategy (BIO-CS) has been recently proposed and illustrated via examples including a nonlinear fermentation process (Lima et al., 2016; Li et al., 2016; and Mirlekar et al., 2017) and a hybrid energy system that integrates different process components (Mirlekar et al., 2017). This approach has shown to have unique features for handling process model nonlinearities as well as flexibility of employing different optimal control solvers and termination criteria when compared to traditional control methods. In case of optimization, techniques that imitate ant colony optimization with improved efficiency have recently been studied under the name of Efficient Ant Colony Optimization (EACO) for molecular design and solvent selection case studies (Gebreslassie and Diwekar, 2015). In addition, the abilities of heuristic-based methods such as EACO, Efficient Genetic Algorithm (EGA) and Efficient Simulated Annealing (ESA) were used to develop homogenous Multi-agent Optimization (MAO) techniques by establishing communication protocol between the algorithm procedures and the global information sharing environment (Gebreslassie and Diwekar, 2015). However, the combination of biomimetic control strategies and agent-based optimization methods for nonlinear systems have not yet been addressed in an integrated fashion. In particular, in the context of process systems engineering, control studies are necessary to address setpoint tracking, disturbance rejection and plant-model mismatch challenges associated with process dynamics. Additionally, optimization plays an important role in identifying the optimal steady states or operating conditions for the processes that will satisfy the overall process objective (e.g., economic, productivity). To fill this gap and combine process control and optimization techniques, in this article, BIO-CS is integrated with MAO to design a novel framework that leads to optimal dynamic process operations. The proposed combination results in a unique biomimetic framework for optimal control of nonlinear chemical processes. In summary, the developed framework yields optimal setpoints or a trajectory of setpoints for a nonlinear, multivariable system considering an overall process objective by employing MAO. This system is then optimally controlled by BIO-CS to achieve the desired output setpoints.

The applicability of the proposed method is demonstrated using a fermentation process model (Li et al., 2016) for bioethanol

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production. The presence of steady-state multiplicities and nonlinearities in this process model poses major challenges for process control and optimization. In particular, in this multivariable system, finding the optimal setpoint associated with production rate (or profitability) and the simultaneous control of product concentration and temperature of the fermentor are critical for optimal performance. The proposed framework is implemented for the fermentation process to address these challenges. Specifically, scenarios of setpoint tracking and plant-model mismatch are considered. The results of the developed method are compared to a gradient-based Sequential Quadratic Programming (SQP) technique (Diwekar, 2008) and a classical proportional-integral (PI) controller in terms of optimization and control studies, respectively.

The rest of the article is organized as follows: Section II presents the proposed concepts including the algorithm details; Section III describes the fermentation process application; Section IV contains the optimization and control results; and Section V presents the conclusions.

2. BIOMIMETIC CONTROL STRATEGY INTEGRATED WITH MULTI-AGENT OPTIMIZATION

2.1 *Proposed Integrated Framework*

The proposed framework for the integration of the BIO-CS controller with the multi-agent optimizer considering process systems applications is shown in Fig. 1. As depicted in this figure, for a given process, the MAO acts in a supervisory layer that considers the minimization or maximization of an overall objective for the whole process. As a result of this optimization, the optimal setpoints or trajectory of setpoints are obtained for the controlled/output variables in different control loops that represent sections of the process simulation. After this optimization, BIO-CS controllers are designed for the coupled control loops to take the process to these desired/optimal operating setpoints. In the particular case of optimization, the MAO search for decision variables in a solution space and then implement those solutions on the process. Note that the process model in this step is only employed to simulate the process and calculate the objective function values. The interaction between the MAO and the process simulation is depicted in Fig. 1 (upper part). The same model, or a reduced version of it, may be used for the design of the model-based BIO-CS controllers. Specifically, as shown in Fig. 1 (lower part), the BIO-CS compute and implement optimal control laws on the process simulation for simultaneously tracking the multiple outputs of the process to their desired setpoints. For a given dynamic system model, it is assumed that the process control loops have been already identified through control structure selection techniques. These control loops or islands are thus simultaneously controlled using BIO-CS and integrated optimally through the MAO approach. The proposed framework is developed in MATLAB by employing in-house MAO and BIO-CS algorithms. Also, the MATLAB function *ode*15*s* is used for process simulation purposes. A schematic with the algorithm details associated with this integrated framework is depicted in Fig. 2. The two main components of the proposed framework (MAO and BIO-CS) are discussed in the next subsections.

2.2 *Multi-agent Optimizer*

The design of the multi-agent optimization approach for process systems applications is explained here in details. In particular, homogeneous MAO techniques are considered for implementation purposes in this paper. Inside homogeneous MAO, multiple agents compute solutions for the optimization problem. The developed MAO routine involves the following steps (depicted in Fig. 2, inside red dotted rectangle):

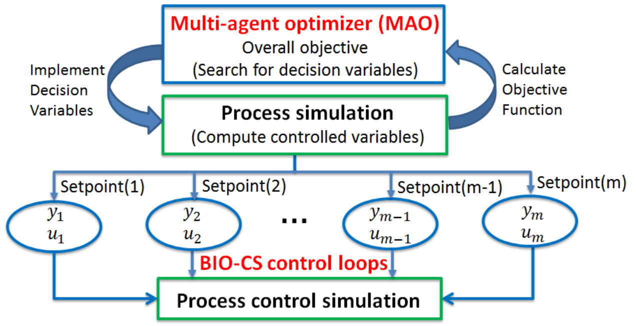

Fig. 1. Schematic of the overall integrated framework of BIO-CS with multi-agent optimization

(*i*) Select MAO algorithm from the available pool (EACO, EGA, ESA, SQP) based on the user's choice (e.g., EACO);

(*ii*) Define parameters for the algorithm initialization;

(*iii*) Generate multiple agents (1, 2, ..., z) of the selected algorithm to obtain solutions for the decision variables by exploiting the capabilities of the chosen algorithm representing each agent;

(*iv*) Simulate the process using the solution of the decision variables obtained from previous step for each agent and compute objective function values;

(*v*) Share the information among the agents globally for coordination and comparison of the obtained solutions;

(*vi*) Check the optimality criteria (e.g., tolerance for the objective function value difference at consecutive iterations);

(*a*) If satisfied, then the MAO converged to an optimal solution;

(*b*) If not satisfied, then repeat steps (*ii*)-(*vi*) by defining different parameters for the agents.

The obtained optimal solution corresponds to the setpoints or trajectory of setpoints for the outputs of the process that can then be used in the implementation of the BIO-CS controllers. Note that in this framework the agents/algorithms involved in the optimization are only dependent on the process model for the calculation of the objective function values. The MAO parameters are independent of the process simulation. The model dependency particularly associated with step (*iv*) of the algorithm is further described next. The mathematical formulation of the optimization problem for process applications is given by,

$$\begin{aligned} \text{minimize} \quad & J = \sum_{i=1}^{k} h(y_i, u_i) \\ \text{subject to,} \quad & u^{lb} \leq u_i \leq u^{ub} \\ \text{in which,} \quad & x_{i+1} = f(x_i, u_i) \\ & y_i = g(x_i, u_i) \end{aligned}$$

in which $u \in \mathbb{R}^m$, $x \in \mathbb{R}^n$ and $y \in \mathbb{R}^p$ are the input, state and output variables, respectively. f and g represent the nonlinear models relating the state, output and input/decision variables of the process in consideration. In the definitions of the inequality

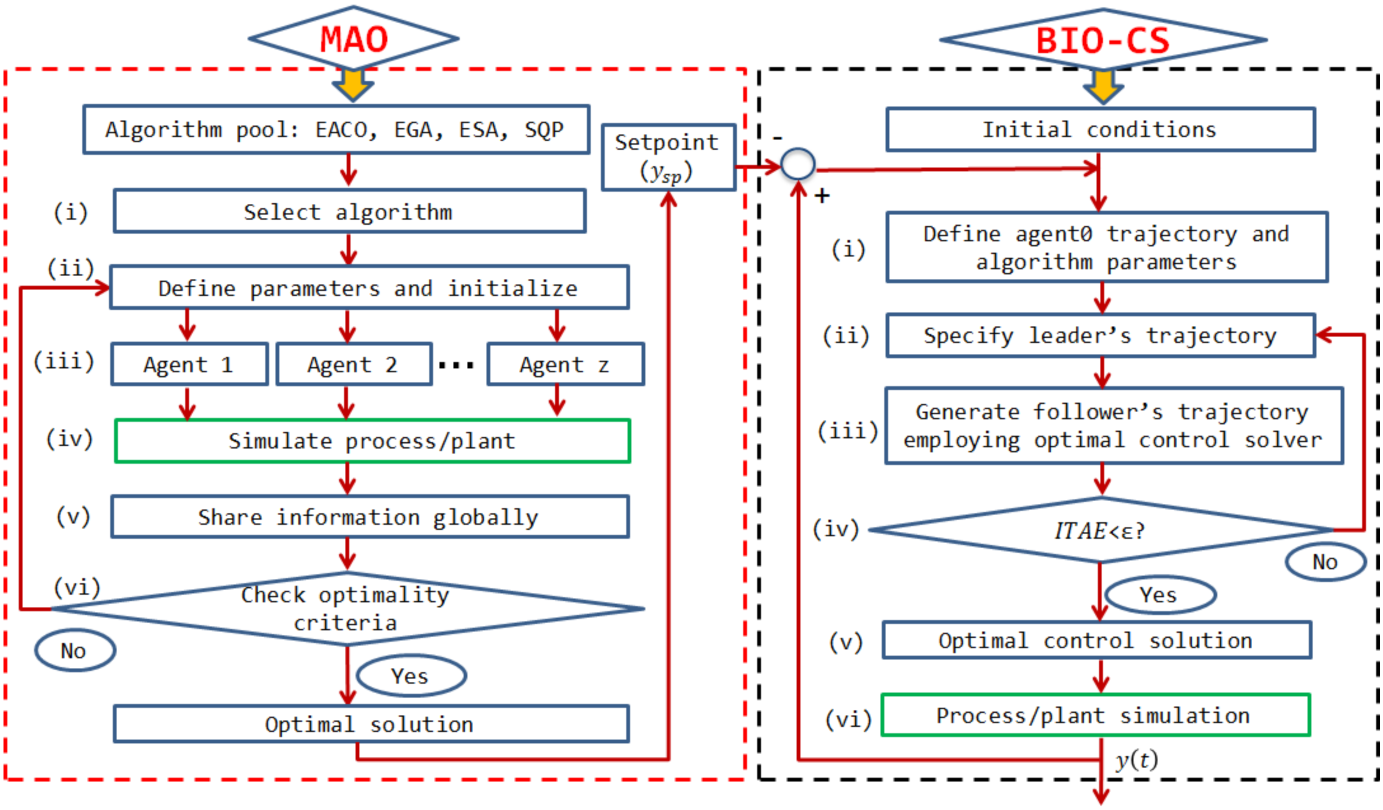

Fig. 2. Schematic of the algorithm details for the integrated BIO-CS with MAO framework

constraints, lb and ub stand for lower and upper bounds, respectively. J denotes the objective function that consists of the summation of the function of the i discrete controlled/output variables over the predefined time horizon with k symbolizing the number of discretization points. The solution of this nonlinear optimization yields the values of the y variable that are feasible to satisfy the optimized objective function for a given time horizon. The first step in the implementation for a process model consists of the selection of decision variables (u) and the number of intervals for discretization (k) for the time horizon. The number of intervals is chosen based on the tradeoff between desired computational efficiency and accuracy. The next step is to discretize the selected decision variable ranges based on the number of intervals. Then, the decision variable values at the discretization points are computed by the optimizer agents based on the algorithm capabilities. Subsequently, the values of the variables involved in the objective function are obtained from the process simulation by implementing the decision variable values computed by the agents at each discretization point. The objective function values at each discretization point are then added together to provide a cumulative J value which is further used in subsequent steps of the algorithm for information sharing and checking the optimality criteria. The mathematical details on the homogeneous MAO that utilizes the potential of multiple agents in terms of coordination, parallelization and diversity by global information sharing can be found in the literature (Gebreslassie and Diwekar, 2017).

2.3 BIO-CS Controller

In this subsection, the BIO-CS algorithm employed for process control applications is discussed. This model-based controller mimics the ants' rule of pursuit idea by combining gradient-based optimal control and agent-based concepts in an intelligent manner. In this control strategy, the agents follow simple rules of interaction that result in optimal control trajectories. The BIO-CS involves the following steps (also depicted in Fig. 2, inside black dotted rectangle):

(i) Start with initial conditions for a given dynamic process model and generate an initial feasible input trajectory (corresponding to an initial guess for agent0). Then select the BIO-CS agents' interaction parameters such as pursuit time ($\triangle$), discretization time (δ) and sampling time (T);

(ii) Specify the obtained trajectory as the leader agent trajectory;

(iii) Generate the follower agent trajectory by employing optimal control solvers (e.g., gradient-based solver) in an intelligent manner. The follower agent communicates with the leader by predefined algorithm parameters to compute its own trajectory;

(iv) Compute the Integrated Time Absolute Error (ITAE) for the follower trajectory over a user defined period of time and then check if this ITAE value lies within a certain threshold (ε);

(a) if yes, the BIO-CS converged to an optimal control solution;

(b) If no, then specify current follower trajectory as the next leader and repeat steps (ii) - (iv).

(v) Retain the optimal control/input profile from BIO-CS for implementation over a predefined sampling time horizon;

(vi) Simulate the process by employing the obtained control laws for a sampling time horizon and then send the feedback signal containing current outputs ($y(t)$) from the process to update the conditions for the next sampling period and close the loop.

For the implementation of BIO-CS on multivariable control loops, the optimal control problem is defined as follows:

$$
\begin{aligned}
&\underset{u(t)}{\text{minimize}} && \varphi = \int_{t_i}^{t_f} \|(y(t) - y_{sp})\|^2 + \|(u(t) - u^-(t))\|^2 dt \\
&\text{such that,} && \dot{x}(t) = f(x(t), u(t)) \\
& && y(t) = g(x(t), u(t)) \\
&\text{subject to,} && x(t)^{lb} \leq x(t) \leq x(t)^{ub} \\
& && u(t)^{lb} \leq u(t) \leq u(t)^{ub}
\end{aligned}
$$

in which the optimal control objective function, denoted by φ, is minimized over a period of time. Here, t_i and t_f are the initial and final times, respectively. The descriptions of the other symbols are mentioned in the previous subsection. The objective function (φ) generally consists of simultaneously maintaining multiple outputs at their desired setpoints, y_{sp}, with the addition of the input suppression term that considers past input moves, $u^-(t)$. These terms are minimizations of the squared errors between the variables and their desired/past values. Thus, the solution of this optimal control problem provides optimal trajectories for each input of the Multi-Input-Multi-Output (MIMO) system addressed to satisfy the objective function and constraints. More details on the design of this controller can be obtained from the literature (Mirlekar et al., 2017). Next, the case study for the implementation of the integrated framework on a nonlinear system considering a fermentation process as an example is explained.

3. NONLINEAR PROCESS CASE STUDY

To demonstrate the applicability of the proposed framework to a nonlinear chemical system, an extension of the fermentation process example presented in reference (Mirlekar et al., 2017) was employed as the implementation case study. For the model extension, to prevent ethanol (end-product) inhibition and improve the productivity and efficiency of the fermentation process, an in situ ethanol-removal membrane is used so that the ethanol is removed as it is being produced. The extended mathematical model also takes into consideration the temperature effect on kinetics parameters, mass and heat transfer, in addition to the kinetic equations modified from the indirect inhibition structural model developed in the literature. In summary, the fermentation process model comprises of seven Ordinary Differential Equations (ODE) and two Algebraic Equations (AE) (see details in Li et al., 2016). The main challenge of this system lies in the nonlinearities for control and optimization studies. For implementation purposes, a MIMO control structure that consists of a two-input-two-output system is chosen from this process. Selected model equations showing the input-output relationships relevant to this paper are given below:

$$\frac{dC_P}{dt} = \frac{P(f(T))(C_S C_e)}{Y_{PX}(K_s + C_S)} + m_p C_X + D_{in} C_{P0} - D_{out} C_P - \frac{\alpha(C_P - C_{PM})}{V_F} \tag{1}$$

$$\frac{dC_{PM}}{dt} = \frac{A_M P_M (C_P - C_{PM})}{V_M} + D_{m,in} C_{PM0} - D_{m,out} C_{PM} \tag{2}$$

$$\frac{dT_r}{dt} = D_{in}(T_{in} - T_r) + f(C_X) f(T_r) - K_F(T_r - T_j) \tag{3}$$

$$\frac{dT_j}{dt} = D_{j,in}(T_{w,in} - T_j) + K_j(T_r - T_j) \tag{4}$$

$$D_{m,out} = D_{m,in} + \frac{A_M P_M (C_P - C_{PM})}{V_M \rho_r} \tag{5}$$

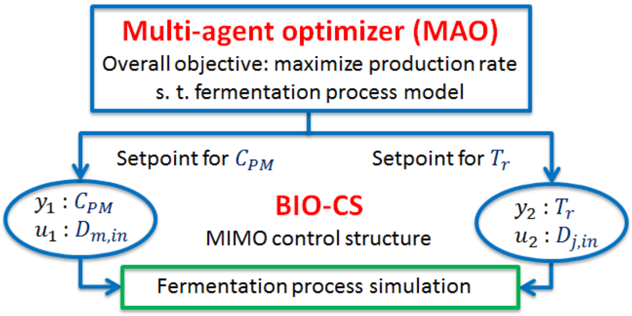

Fig. 3. Schematic of the integrated framework with BIO-CS and multi-agent optimization for the fermentation process

in which, equations (1) and (2) represent the mass balances for the product concentration on the fermentor side (C_P) and membrane side (C_{PM}), respectively. These equations also relate concentrations of other species involved in the reaction system in the fermentor, such as biomass (C_X), key component (C_e) and substrate (C_S). Equations (3) and (4) show the energy balance in terms of temperature of the fermentor (T_r) and the jacket (T_j), respectively. The remaining equation (5) is the algebraic equation considered in this fermentation process model in which the parameter $\alpha = A_M P_M$. The definitions of all the constants and parameters involved in this model and their nominal values were obtained from the literature (Li et al., 2016) and are summarized in Table 1.

Table 1. Base case set of constants and parameters used for the fermentation process model

Parameter	Description	Value
C_{P0}	Inlet fermentor product concentration (kg/m^3)	0.01
C_{PM0}	Inlet membrane product concentration (kg/m^3)	0.01
D_{in}	Inlet fermentor dilution rate (h^{-1})	0.1
D_{out}	Outlet fermentor dilution rate (h^{-1})	0.1
$D_{m,in}$	Inlet membrane dilution rate (h^{-1})	0.5
$D_{m,out}$	Outlet membrane dilution rate (h^{-1})	0.5
$D_{j,in}$	Inlet cooling water dilution rate (h^{-1})	0.5
T_{in}	Inlet temperature of reactants (^oC)	30
$T_{w,in}$	Inlet temperature of cooling water (^oC)	28
K_s	Monod constant (kg/m^3)	0.2
K_F	Heat transfer constant (h^{-1})	1.8324
K_j	Heat transfer constant (h^{-1})	0.0714
m_p	Maintenance factor based on product (kg/kgh)	1.1
Y_{PX}	Yield factor based on product (kg/kg)	0.0526
V_F	Fermentor volume (m^3)	0.003
V_M	Membrane volume (m^3)	0.0003
P	Maximum specific growth rate (h^{-1})	1.0
ρ_r	Reactants density (kg/m^3)	1080
P_M	Membrane permeability (m/h)	0.1283
A_M	Area of membrane (m^2)	0.24

In this paper, the membrane dilution rate, $D_{m,in}$, as well as the cooling water dilution rate in the jacket, $D_{j,in}$, are chosen as the manipulated variables for the regulation of ethanol concentration, C_{PM}, and fermentor temperature, T_r, respectively. The bound constraints on the manipulated variables are placed as $0 \leq D_{m,in}, D_{j,in} \leq 1.5$. The selected control loops for the fermentation process representing multiple islands along with their integration using multi-agent optimization is depicted in the schematic in Fig. 3. In the next section, the MAO analysis and the BIO-CS implementation results for setpoint tracking and plant-model mismatch scenarios are discussed.

4. IMPLEMENTATION RESULTS

4.1 Multi-agent Optimization Results

For the implementation of the multi-agent optimizer to address the fermentation process, the manipulated variables associated with the control loops, i.e., $D_{m,in}$ and $D_{j,in}$ are selected as the decision variables. Also, the time horizon for the optimization is chosen to be 20 h with the length of intervals of 4 h each. This results in 5 discretization points for each of the decision variables excluding the initial point. Inside the optimizer, agents are employed to calculate the values of these decision variables at each discretization point and implement those values in the process simulation using $ode15s$ in MATLAB. From this process simulation, the objective function values as a function of the controlled and decision variables are computed for each corresponding discretization point. These discrete values are then combined to calculate the cumulative objective function value. For the implementation of the homogeneous MAO, an optimization problem is formulated considering an overall objective of maximization of production rate, J, which is related to the system profit, defined as follows,

$$\text{maximize} \quad J = C_P D_{out} V_F + C_{PM} D_{m,out} V_M$$

It is important to note that J is a function of three variables that are associated with state/decision variables of the system (C_P, C_{PM} and $D_{m,out}$). The implementation results of the homogeneous MAO technique with EACO, EGA and ESA as the selected algorithms for the fermentation process are summarized in Table 2. Note that each selected homogeneous MAO only considers agents with similar features, i.e., agents differ only in terms of the algorithmic parameters and the initialization. These results are also compared to the gradient-based SQP (employing $fmincon$ with its default parameters in MATLAB) considering the same parameters and the result is also given in Table 2. The cumulative J values in case of heuristic-based

Table 2. MAO implementation results

Outputs	EACO	EGA	ESA	SQP
C_{PM} (kg/m^3)	36.87	37.00	36.90	37.01
T_r (^oC)	28.66	28.84	28.84	28.67
J (kg/h)	0.1252	0.1252	0.1252	0.1183
$CPU\ time$ (s)	332.14	4941.82	6086.31	24.94

MAO approaches are on average 5.5% higher than their SQP counterpart, which could result in significant economic benefits in the long run. The agents of each MAO technique search the solution space for decision variables extensively using their own capabilities that leads to the optimal value for the objective function. However, the computational time efficiency of the SQP implementation is higher due to the probabilistic sampling used for the solutions in case of heuristic-based methods vs. the directional search method employed in the gradient-based approach (SQP). Such longer computational time should not be an issue if the MAO is running offline multiple times or periodically during process operation, especially for this biochemical system with a time scale in order of hours. Given the performance vs. computational time tradeoff, the obtained optimal setpoint values from homogeneous MAO with multiple EACO as algorithmic agents are selected. Specifically, the controlled variable values obtained at the end of the optimization time horizon as shown in Table 2 are supplied as setpoints for the control studies. Next, the closed-loop controller implementation results with these setpoints are discussed.

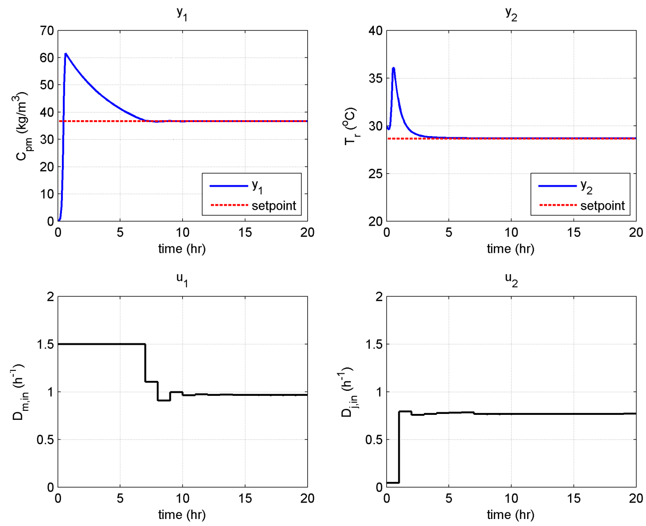

Fig. 4. BIO-CS simulation for setpoint tracking: (a) output (y_1); (b) output (y_2); (c) input (u_1); and (d) input (u_2) trajectories

4.2 Closed-loop Control Results: Setpoint Tracking

The implementation results of the BIO-CS controllers that are designed for the selected control loops are discussed here. The goal of the BIO-CS controllers is to take the system to the optimal setpoints obtained from the MAO calculations. The BIO-CS implementation results for the chosen control structure are shown in Fig. 4. The BIO-CS parameters considered for this implementation are: pursuit time ($\triangle$) of 1 h, discretization time (δ) of 0.1 h and threshold value (ε) of 0.1. The setpoints for C_{PM} of 36.87 kg/m^3 and T_r of 28.66 ^oC are selected from the results of homogeneous MAO with EACO as multiple agents. As depicted in Fig. 4, BIO-CS provides optimal control trajectories that reach the desired output setpoints within 9 h for C_{PM} and 4 h for T_r successfully with smooth input profiles. The comparison of the obtained results with classical PI controllers are considered next. The PI controller results (obtained by extensive trial and error tuning) depicted in Fig. 5 display slower and oscillatory response with slightly higher overshoot for C_{PM} compared to the BIO-CS implementation. In particular, the product concentration on the membrane side reach the steady-state shortly after the simulation time horizon of 20 h. The observed oscillations translate to production rate losses due to operation away from the optimal conditions. Specifically, the cumulative production rate calculated is approximately 15% higher for the BIO-CS implementation when compared to the PI controller. Thus, the BIO-CS implementation brings the system to its desired setpoints in an optimal manner with reduced overshoot when compared to the PI controller performance.

4.3 Closed-loop Control Results: Plant-Model Mismatch

The next case is simulated considering a plant-model mismatch scenario. In particular, the constant Y_{PX} is changed in the plant model, but not in the controller model thus affecting the process outputs as depicted in equation (1). Specifically, the value of Y_{PX} is increased from 0.0526 to 0.0631 kg/m^3 which is approximately a 20% change from its original value. This scenario essentially simulates the effect when increasing the yield factor based on product, affecting the product concentration of the fermentation process. Initially, without re-running the MAO, the BIO-CS controller with plant-model mismatch is implemented by using the setpoints from the previous case study.

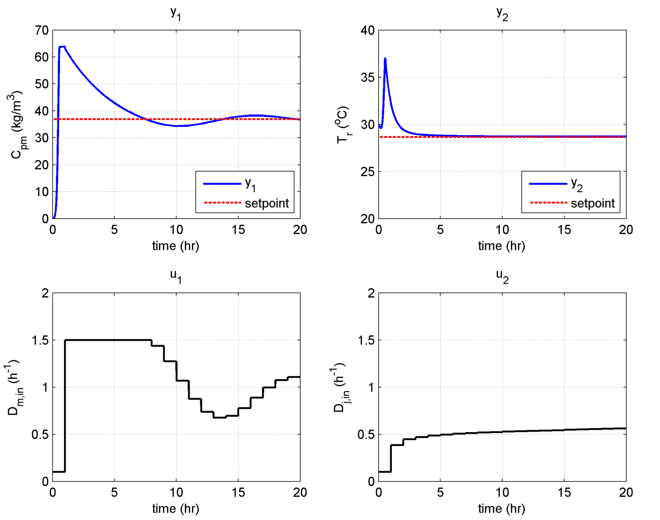

Fig. 5. PI simulation for setpoint tracking: (a) output (y_1); (b) output (y_2); (c) input (u_1); and (d) input (u_2) trajectories

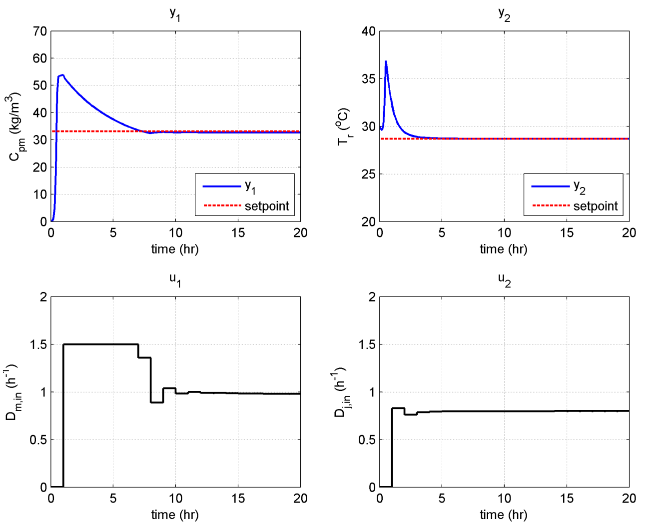

Fig. 6. BIO-CS simulation for plant-model mismatch: (a) output (y_1); (b) output (y_2); (c) input (u_1); and (d) input (u_2) trajectories

For this scenario, the cumulative production rate now considering the mismatch over the given time horizon is calculated to be approximately 0.1001 kg/h. Due to such mismatch, this production rate of the system is no longer optimal. Therefore, the MAO is re-run to obtain the optimal operating conditions that maximize the system production rate and then the BIO-CS is implemented to mitigate the effect of the model mismatch for providing optimal system performance for the new conditions. In practice, MAO would run periodically or even online depending on the process time scale. For homogeneous MAO with EACO agents, the values of the optimal setpoints for C_{PM} and T_r are obtained as 33.13 kg/m^3 and 28.67 ^oC, respectively, with maximum cumulative production rate of 0.1109 kg/h. The optimal cumulative production rate obtained from MAO is on average 10% higher than the case without re-running MAO, which would result in loss of productivity that translates into reduced profit. The BIO-CS implementation results shown in Fig. 6 illustrate the successful performance. Therefore, the proposed integrated framework of BIO-CS with MAO is able to tackle the additional challenges imposed on the process successfully.

5. CONCLUSIONS

In this article, the BIO-CS algorithm was integrated with MAO for implementation on nonlinear, multivariable processes to obtain optimal system performance. Specifically, a multivariable control structure derived from a nonlinear fermentation process example was addressed. The results of the homogeneous MAO considering an agent pool of heuristic-based algorithms such as EACO, EGA and ESA were compared to a gradient-based SQP method in terms of objective function value and computational time efficiency. In addition, BIO-CS control studies using the outcome of MAO were performed for the process considering setpoint tracking and plant-model mismatch scenarios. The BIO-CS controller showed superior performance to that of the classical PI controller in terms of improved and faster responses. The performed studies provide an integrated approach for biomimetic agent-based control with optimization methods that can be employed in a variety of process systems engineering applications. The proposed framework provides an alternative for the typical Real-time Optimization (RTO) combined with Model Predictive Control (MPC) setup considering different optimization algorithms. The fundamental comparison of BIO-CS with MPC in terms of how BIO-CS is cast as an MPC will be subject of future investigation. Also, the implementation of BIO-CS for other energy systems will be investigated.

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