Optimizing the Open-and Closed-Loop Operations of a Batch Reactor

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Abstract—The purpose of this paper is to optimize the function of a batch reactor operating in open and closed loops. A simultaneous optimization method is employed. This optimization method provides optimal solution at a finite number of points in time. However, the actual batch reactor operation may deteriorate if the computed optimal input is improperly applied to the process. In the open-loop operation, an appropriate wave-shaping method is employed to modify the computed optimal discrete input profile to achieve an improved batch operation while simultaneously guaranteeing the enforcements of the path and end-point constraints. In the closed-loop operation, to improve the disturbance rejection capability of the reactor, two optimizer structures based on the nonlinear model predictive control (NMPC) are developed. The first structure is founded on a modified version of a conventional approach which utilizes a variable number of finite elements (VNFE). The second optimizer introduced in this paper is a newly developed scheme which is compared against the first approach. This approach makes use of a variable number of collocation points (VNCP). Simulation studies, considering both of the fixed batch-time problem (FBTP) and minimum batch-time problem (MBTP), are presented in this paper.

Index Terms—batch reactor, dynamic optimization, path and end-point constraints, nonlinear model predictive control

I. INTRODUCTION

Batch reactors are broadly used in the manufacturing of fine chemicals and other expensive products. In a batch reactor, there are no feed and output product flows while the reaction is being performed. This is an intrinsically unsteady-state operation where temperatures and concentrations dynamically alter with time.

The dynamic optimization of batch processes in recent years [1]-[8] has become an accepted choice for reducing production costs, enhancing product quality, meeting protection requirements and satisfying environmental regulations. The dynamic optimization problem has path and end-point constraints which result in a complex optimization problem.

A commonly used approach to achieve dynamic optimization is known as the simultaneous optimization technique. The major feature of the simultaneous optimization technique is the fact that the optimization is performed in the space of discretized inputs and states. Therefore, the dynamic equations and discretized constraints of the system are valid only at a limited number of time instants.

In the open-loop batch operations considered in this work, it has been demonstrated that the shape of the manipulating input, constructed using the computed discrete points of the input trajectory, brings about different process responses.

Because of the lack of process measurements, the open-loop batch operations are extremely influenced by the disturbances and model mismatch. If quick response to a disturbance is required, process measurements are fed back to the system and repeated optimizations are implemented online [10]-[15]. This paper introduces a new scheme to improve the disturbance rejection capability of the batch reactors operating in a closed-loop implementation.

In the following section, we describe the process and the modelling steps using the first principles equations. Optimization of batch processes and the simultaneous optimization method are reviewed in Section III. In Section IV, the use of dynamic optimization in open-loop operations is portrayed. In this section, a method is proposed to improve the reactor operation. In Section V, two developed online optimization methods are described. Finally, the results obtained are illustrated in Section VI.

II. MODELLING OF BATCH REACTOR

An illustration of the reactor is shown in Fig. 1. In the vessel, strongly exothermic successive reactions are presumed to take place. Component A is consumed by chemical reaction producing the product B. Component B further reacts to the undesired by-product C:

\[ A \rightarrow^{k_1} B \rightarrow^{k_2} C \]  

where \( k_1 \) and \( k_2 \) are rate constants.

The reactor is equipped with a cooling system, a jacket around the reactor vessel. Aziz and Mujtaba [16] investigated both a simple and a detailed model of this reaction system. The detailed model is considered here.

A chemical process can mathematically be described by mole and energy balances, resulting in a differential-algebraic equation (DAE) system. The mole balances for the constant-volume reactor give:
\[
\frac{dc_a}{dt} = -2k_1c_a \\
\frac{dc_b}{dt} = k_1c_a - k_2c_b \\
\frac{dc_c}{dt} = k_2c_b
\]

where \(C_a, C_b,\) and \(C_c\) are the concentrations of components (kmol/m\(^3\)). The temperature dependence of the rate constants follows the Arrhenius rate law:

\[
k_i = k_{i,0} \exp \left( -\frac{E_i}{RT} \right) \quad i = 1,2
\]

where \(k_{i,0}\) and \(E_i\) are the pre-exponential constants (4.38 \times 10^4 and 3.94 \times 10^6 \text{ h}^{-1},\) respectively); \(E_1\) and \(E_2\) are the activation energy constants (3.49 \times 10^7 and 6.50 \times 10^8 \text{ J kmol}^{-1}\); \(R\) is the universal gas constant (8314 J kmol\(^{-1}\) K\(^{-1}\)); and \(T\) is the temperature (K).

The energy balances for the model are:

\[
\frac{dT}{dt} = \frac{Q - Qm}{Cp_mV} \\
\frac{dT_m}{dt} = \frac{Qm - Ql}{Cp_mV_mV\rho_m} \\
\frac{dT_j}{dt} = \frac{V_i}{V_j}(T_{j,0} - T_j) + \frac{Q_l}{Cp_iV_i\rho_j}
\]

\[
Q_r = -\Delta H_1(k_1C_aV) - \Delta H_2(k_2C_bV)
\]

\[
Q_m = U_jA_j(T - T_m)
\]

\[
Q_j = U_aA_0(T_m - T_j)
\]

where \(T_m\) is the metal temperature (K); \(T_j\) is the coolant temperature (K); \(Q\) is the heat of reaction (J h\(^{-1}\)); \(Q_m\) is the heat transfer to metal (J h\(^{-1}\)); \(Q_l\) is the heat to coolant (J h\(^{-1}\)); \(C_p\) is the reactant specific heat (4200 J kg\(^{-1}\) K\(^{-1}\)); \(C_{p_m}\) is the specific heat of reactant (500 J kg\(^{-1}\) K\(^{-1}\)); \(C_{p_i}\) is the specific heat of the coolant (800 J kg\(^{-1}\) K\(^{-1}\)); \(\rho_m\) is the density of the metal (8200 kg m\(^{-3}\)); \(\rho_i\) is the density of the coolant (1000 kg m\(^{-3}\)); \(V\) is the reactant volume (1.23 m\(^3\)); \(V_m\) is the volume of the metal (0.27 m\(^3\)); \(V_i\) is the volume of the coolant (0.53 m\(^3\)); \(\Delta H_1\) and \(\Delta H_2\) are the reaction enthalpy constants (-6.50 \times 10^8 and -1.20 \times 10^8 J kmol\(^{-1}\)), respectively); \(U_j\) is the inside heat-transfer coefficient (7.0 \times 10^6 J h\(^{-1}\) K\(^{-1}\) m\(^{-2}\)); \(U_i\) is the outside heat-transfer coefficient (8.18 \times 10^6 J h\(^{-1}\) K\(^{-1}\) m\(^{-2}\)); \(A_j\) is the inside heat-transfer area (5.25 m\(^2\)); and \(A_i\) is the outside heat-transfer area (5.25 m\(^2\)).

It is assumed [16] that the system is preheated to 350 K and the jacket is filled with water at 300 K. The initial conditions are: \(C_{a}(t_0) = 0.975; C_{b}(t_0) = 0.025; C_{c}(t_0) = 0; T(t_0) = 350\) K; \(T_m(t_0) = 373\) K; and \(T_f(t_0) = 300\) K.

### III. DYNAMIC OPTIMIZATION OF THE BATCH REACTOR

#### A. The FBTP

In the FBTP, with a specified final batch time, \(t_b\), and dynamic model equation, \(f\), the desired product concentration, \(x_{d}\), is maximized as:

\[
\text{max}_{x_{d}} x_{d}(t_b)
\]

s.t.

\[
\dot{x} = f(x, F_j, p), \quad x(t_0) = x_0
\]

\[
0 < F_j(t) < F_U \\
T(t) < T_U \\
T(t_b) < T_f \\
x_W(t_b) < x_Wf
\]

where \(x(t)\) is an n-dimensional state vector; \(p\) is a parameter vector; \(F_j\) is the coolant flow; \(F_U\) is the upper bound of the coolant flow; \(x_W\) is the waste; \(x_Wf\) is the end-point concentration for the waste; \(T_U\) is the upper bound of the reactor temperature; \(T_f\) is the end-point temperature of the reactor; and \(t_0\) is the initial time.

For the process described in Section II, \(x = [C_{a} C_{b} C_{c} T, T_m, T_j]; x_d = C_b;\) and \(x_u = C_c\).

#### B. The MBTP

In the MBTP, the optimization objective is to minimize the batch time required to satisfy some performance specifications such as to obtain a required end-point concentration value, \(x_{f}\), for \(x_{d}\), by manipulating the coolant flow rate as:

\[
\text{min}_{t_b} f_j
\]

s.t.

\[
\dot{x} = f(x, F_j, p), \quad x(t_0) = x_0
\]

\[
0 < F_j(t) < F_U \\
T(t) < T_U \\
T(t_b) < T_f \\
x_W(t_b) < x_Wf
\]

\[
x_d(t_b) = x_f
\]

For the process described in Section II, \(x_f = C_{by}\)

In a time optimal problem it is in the interest of the chemical process industry to shorten the batch time and to drive the processes closer to their real constraints.

\[\text{Figure 1. A jacketed batch reactor.}\]

### C. Method of Simultaneous Optimization

The main characteristic of the simultaneous approach is the fact that the optimization is carried out in the space of discretized inputs and states. Here, the inputs and the states are parameterized using a finite number of decision variables. The differential equations are discretized via orthogonal collocation [9]; therefore, the differential equations are satisfied only at a finite number of time steps.
instants. These steps lead to a standard nonlinear programming problem (NLP) which is solved using a method such as the successive quadratic programming (SQP). Thus, in general, the dynamic equations and the discretized constraints are satisfied at the solution of the optimization problem only.

IV. OPEN-LOOP REACTOR OPERATION

In the open-loop reactor operation the optimization is merely carried out at the start of the batch time. Then the control input computed by the optimization algorithm is applied to the process for the duration of the batch time. No process measurement is performed to modify the control input during the batch time.

In the simultaneous optimization approach described in Subsection III.C, the optimization is carried out in the space of discretized variables. This means that the discretized constraints are in general satisfied at the solution of the optimization problem only. Therefore, the shape of the waveform connecting the computed discrete points of the input trajectory may lead to different process responses. In this project, the control input applied to the process can either be in the form of a rectangular pulse or a multi-stage staircase waveform. The durations of these two waveforms extend from any two consecutive points (boundary or collocation) on the finite elements. For the multi-stage staircase input, these durations are divided into Nsteps number of equal steps. The manipulating input is assumed to be constant during each step.

Due to the lack of process measurements during the batch time, the process response is highly affected by the disturbances and model mismatch.

V. CLOSED-LOOP REACTOR OPERATION

A. Closed-Loop Method based on the VNFE (CLVNFE)

If rapid response to a disturbance is needed, the optimal profiles must be re-evaluated online. The online optimization, CLVNFE, employs a modification of the scheme known as the shrinking horizon NMPC described in Diehl et al. [10], Eaton & Rawlings [11], Liotta et al. [12], Soni & Parker [13], and Thomas et al. [14]. In this method, the batch time is divided into a number of equal steps. For the multi-stage staircase input, these durations are divided into Nsteps number of equal steps. The manipulating input is assumed to be constant during each step.

Due to the lack of process measurements during the batch time, the process response is highly affected by the disturbances and model mismatch.

VI. RESULTS

A. Optimization and Open-Loop Results for the FBTP
In the FBTP, the objective is to maximize the conversion of the desired product B. In the reaction, an end-point constraint for the reactant temperature (\(T \leq 320\) K) is imposed to guarantee that the products are at or below certain desired temperature. The total batch time is fixed and equal to 4 h and the number of finite elements, \(n_x\), is 2. Coolant flow is bounded between 0 m\(^3\)/h (valve fully closed) and 9 m\(^3\)/h (valve fully open). The end-point inequality constraint for the waste (product C) is set to 0.10. The reactor temperature must not exceed 360 K at any time (path constraint). Number of collocation points on each finite elements of \(u\), \(N_{colu}\), and number of collocation points on each finite element of \(x\), \(N_{colx}\), both are equal to five.

Fig. 2 shows the concentration profile of the raw material \(C_a\), the concentration profile of the desired product \(C_b\), the concentration profile of the by-product \(C_c\), the reactor temperature profile \(T\) and the optimal coolant profile \(F_j\). From this figure, the value of the achieved conversion to the desired product \(C_b(t_b) = 0.637\), the end-point concentration for the waste \(C_c(t_b) = 0.098\) and the end-point reactor temperature \(T(t_b) = 320\) K. These results clearly show that the two end-point constraints and the path constraint are satisfied.

![Plots of the optimization run](image)

Figure 2. The optimization results for the reactor model (FBTP, \(N_{colu} = 5\), \(N_{colx} = 5\), \(n_x = 2\)).

The computed optimal control input in Fig. 2 is applied to the process. The control input applied to the process is taken to be in the form of a rectangular pulse. The duration of the pulse extends from any two consecutive optimal points (boundary or collocation) on the finite elements. Fig. 3 shows the output profiles for \(C_a\), \(C_b\), and \(C_c\); the profiles for the output \(T\) and input \(F_j\). From this figure the values for \(C_b(t_b) = 0.663\), \(C_c(t_b) = 0.164\) and \(T(t_b) = 338.6\). These results demonstrate that contrary to the results shown in Fig. 2, the end-point constraints and the path constraint are violated. The violations are due to the inherent disadvantage of the simultaneous optimization method (Subsection III.C) used to determine the profiles of Fig. 2.

In this and the following experiments, the path violation error is integrated to obtain the figure \(I_{Err}\) which is used to quantify this violation. For the rectangular control input used in this experiment \(I_{Err}=24.27\). In this case, the increase in the product yield is due to the reactor temperature violation of the path constraint.

In the manipulating input profiles of Figs. 2-13, the real locations of the collocation points within the elements are shown. In Figs. 2 and 7, the computed input profiles are theoretical and are not actually applied to the process. In Figs. 3 and 8 the level of manipulating input between any two consecutive points remains constant; and in Figs. 4-6 and 9-13, the shape of a manipulating input between any two consecutive points is in the form of a multi-level staircase as explained in Section IV.

In Fig. 4, the control input applied to the process is taken to be in the form of a staircase waveform extending between any two consecutive optimal points. The \(N_{steps}\) parameter defined in Section IV is equal to three. Fig. 4 shows the process outputs and input profiles. From this figure the values for \(C_b(t_b) = 0.646\), \(C_c(t_b) = 0.11\), \(T(t_b) = 323.3\) and \(I_{Err} = 5.163\). These results show that the staircase control input improved the performance of the reactor when compared against the rectangular input used in Fig. 3; however, all constraints are still being violated.
In the next experiment, the \textit{Nsteps} parameter is taken to be equal to five and the above experiment is repeated. Fig. 5 shows the process outputs and input profiles. From this figure the values for $C_b(t_0) = 0.624$, $C_c(t_0) = 0.086$, $T(t_0) = 317.2 \, \text{K}$ and $I_{Err} = 0.03$. These results show that the end-point constraints are satisfied and $I_{Err}$, when compared against the previous experiment, is drastically reduced.

The control input shown in Fig. 5 is applied to the process. However, at time $t = 0.9 \, \text{h}$ the process is subjected to a disturbance in the form of $65\%$ reduction in $U_i$. Fig. 6 shows the output and input profiles. From this figure the values for $C_b(t_0) = 0.658$, $C_c(t_0) = 0.140$, $T(t_0) = 331.4 \, \text{K}$ and $I_{Err} = 16.3$. These results indicate that due to the process-model mismatch the end-point constraints and the path constraint are not satisfied.
B. Optimization and Open-Loop Results for the MBTP

In a time-optimal problem the objective is the minimization of the final batch time. The net conversion to the desired product is given. Here, we assumed $C_{bf} = 0.6$, therefore, the end-point equality constraint for the product concentration is set to 0.6. The following MBTP experiment employs the two terminal constraints, the path constraint, bounds, number of finite elements and number of collocation points used in the previous FBTP experiments. However, the MBTP optimizes the control variable in conjunction with the batch time.

Fig. 7 shows the states for the concentrations and the reactor temperature generated by the optimizer. From this figure the values for $C_b(t_b) = 0.6$, $C_c(t_b) = 0.075$, $T(t_b) = 320 \text{ K}$. The optimum batch time is computed to be equal to $t_{op} = 3.406 \text{ h}$. The user is required to specify an initial estimate for the optimum batch time. This value is set to $1.8 \text{ h}$ in our experiment. Similar to the results shown in Fig. 2, these results show that the two end-point constraints and the path constraint are satisfied.

Two additional MBTP experiments are performed using staircase control inputs with $N_{steps} = 1$ and $3$. In each experiment the computed optimal control input in Fig. 7 is applied to the process. Results similar to Figs. 3 and 4 demonstrating violations of the constraints are obtained. Then an experiment, using a staircase control input with $N_{steps} = 5$, is carried out. No disturbance is applied in this case. Fig. 8 shows the input and output profiles. From this figure, the values for $C_b(t_b) = 0.581$, $C_c(t_b) = 0.064$, $T(t_b) = 317.6 \text{ K}$ and $I_{Err} = 0$. All the terminal constraints, the path constraint and bounds are satisfied.
A disturbance as defined in Fig. 6 is then applied to the process. Fig. 9 shows the resulting input and output profiles. From this figure the values for $C_a(t_h) = 0.627$, $C_b(t_h) = 0.1$, $T(t_h) = 333$ K and $I_{Err} = 9.85$. It can be seen that due to the process-model mismatch the terminal and path constraints on temperature are not satisfied. A summary of the results of the experiments performed so far is given in Table I.
The system used to execute the codes in this paper is a microcomputer with AMD 3.0+ GHz CPU, 512M bytes RAM and 512k bytes cache memory. These results indicate that by feeding back the measurements at the sampling points, the end-point constraints are satisfied. Also, for the path constraint, the value of \( I_{Err} = 5.52 \) is smaller than \( I_{Err} = 16.3 \) resulted in Fig. 6. In this experiment, the horizons are decremented at consecutive ORs in order to reduce the computational load and avoid control pulses with undersized extends being computed and then applied to the process.

To enhance the performance of the above experiment, the batch time is divided into 6 identical finite elements (\( N_{max} = 6 \)) each containing two collocation points. The \( N_{steps} \) parameter used in the previous experiment is decremented by one (i.e, \( N_{steps} = 4 \)) to avoid control pulses with undersized extends being applied to the process. The optimization algorithm is invoked six times. In addition, the process measurements take place at \( t = t_b/6, t_b/3, t_b/2, 2t_b/3 \) and \( 5t_b/6 \). Fig. 11. shows the resulting output and input profiles. From this figure the values for \( C_b(t_b) = 0.538, \ C_c(t_b) = 0.045, \ T(t_b) = 306.2 \ K, \ I_{Err} = 2.84 \) and \( t_e = 53.5 \ s. \) These results indicate that by feeding back five sets of process measurements (\( N_{meas} = 5 \)), the end-point constraints are satisfied. Also, for the path

### C. Results for the Online Optimization

1) Results for the online optimization CLVNFE

If reaction to the presented disturbance in Fig. 6 (or in Fig. 9) is necessary, the optimal profiles must be re-calculated online. Here, we use the developed CLVNFE, as described in Subsection V.A. The batch time is divided into five identical finite elements (\( N_{max} = 5 \)) each containing two collocation points. The \( N_{steps} \) parameter defined in Section IV is equal to five. The optimization algorithm is invoked five times. At \( t = 0 \), the first OR utilizes all five finite elements as the prediction horizon and control horizon (i.e., \( PH = CH = 5 \)). At \( t = t_b/5 \), the second OR employs elements 2 to 5 (with \( PH = CH = 4 \)). At \( t = 2t_b/5 \), the third OR employs elements 3 to 5 (with \( PH = CH = 3 \)). At \( t = 3t_b/5 \), the fourth OR employs elements 4 and 5 (with \( PH = CH = 3 \)). Finally, at \( t = 4t_b/5 \) the fifth OR employs element 4 (with \( PH = CH = 1 \)). In addition, process measurements corresponding to the differential variables are taken at \( t = t_b/5, 2t_b/5, 3t_b/5 \) and \( 4t_b/5 \). Fig. 10. shows the output and input profiles. From this figure the values for \( C_b(t_b) = 0.574, \ C_c(t_b) = 0.060, \ T(t_b) = 307.6 \ K, \) and \( I_{Err} = 5.52 \). The computational effort of the whole batch process algorithm \( t_e = 27.2 \ s. \) The system used to execute the codes in this paper is a
constraint, the value of \( I_{Err} = 2.85 \) is smaller than \( I_{Err} = 5.52 \) of the previous experiment. Employing the optimization CLVNFE, two more experiments are carried out using \( N_{imax} = 7 \) and 8 (with \( N_{steps} = 3 \) and 2, respectively). A summary of the results of the four experiments performed in this subsection is given in Table II. It can be seen that a reduction in \( I_{Err} \) is achieved at the expense of an increase in the computational effort and a decrease in the concentration of the desired product.

**TABLE II. CLVNFE (\( N_{col} = 2; \ T_\alpha = 4 \ H; \ \text{DIST.} = -65\%) \)**

<table>
<thead>
<tr>
<th>( N_{imax} )</th>
<th>( N_{steps} )</th>
<th>( N_{max} )</th>
<th>( C_a (t) )</th>
<th>( C_b (t) )</th>
<th>( T (t) ) (K)</th>
<th>( t_s (s) )</th>
<th>( I_{Err} )</th>
<th>( \text{Fig.} )</th>
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<tr>
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<td>0.060</td>
<td>307.6</td>
<td>27.2</td>
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<tr>
<td>7</td>
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<td>6</td>
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<td>0.038</td>
<td>305.8</td>
<td>63.8</td>
<td>1.41</td>
<td>-</td>
</tr>
<tr>
<td>8</td>
<td>2</td>
<td>7</td>
<td>0.502</td>
<td>0.034</td>
<td>305.4</td>
<td>142.6</td>
<td>1.12</td>
<td>-</td>
</tr>
</tbody>
</table>

Figure 10. Closed-loop operation of the reactor using the CLVNFE (\( FBTP, \ N_{col} = 2, \ N_{imax} = 5, \ \text{staircase control input, } N_{steps} = 5 \)).

Figure 11. Closed-loop operation of the reactor using the CLVNFE (\( FBTP, \ N_{col} = 2, \ N_{imax} = 6, \ \text{staircase control input, } N_{steps} = 5 \)).
2) Results for the online optimization CLVNCP

Here, the developed CLVNCP, as described in Subsection V.B is used to react to the presented disturbance in Fig. 6. At this time, two finite elements each of which consisting of an initial maximum number of three collocation points on x and u, Ncol\text{max} are used for the entire batch time. Nsteps is equal to 5. The threshold time gap (defined in Subsection V.B) \( t_g = n_d \text{ac} = 1 \text{ hr} \). Based on this figure, as the experiment is progressed, the number of collocation points on the finite elements is decremented to reduce the computational load and avoid control pulses with undersized lengths being computed and consequently applied to the process. Table III gives a summary of the overall optimization process throughout the batch time. The first row in this table shows the \( OR \) number; the second row gives the starting time of each \( OR \) and the data measurement times; the third row gives the horizon corresponding to each starting time in the second row; and the fourth row gives the number of collocation points of the finite elements. As shown in this table, the batch time consists of three time gaps in each of which the implemented ORs employ the same number of collocation points. The first time gap extends from 0 to 1.007 hr. Four ORs with \( Ncol = 3 \) are performed in this gap. Four sets of measurements (at \( t = 0.225, 0.438, 0.639 \) and \( 0.828 \text{ hr} \)), each of which specifying the values corresponding to the differential variables, are acquired in the first time gap. Two other time gaps start at \( t = 1.007 \) and 2.085 hr. The optimization procedure is invoked thirteen times during the batch time and requires twelve sets of process measurements (\( N_{\text{ meas}} = \text{12} \)).

Fig. 12 shows the output and input profiles for this experiment. From this figure the values for \( C_i(t_b) = 0.602, C_i(t_b) = 0.071, T(t_b) = 314.31 \text{ K}, I_{\text{ Err}} = 0.76 \) and \( t_e = 24 \text{ s} \). These results indicate that by feeding back twelve sets of process measurements, the end-point constraints are satisfied. Also, for the path constraint, the value of \( I_{\text{ Err}} = 0.76 \) is smaller than \( I_{\text{ Err}} = 5.52 \) resulted in Fig. 10 and \( I_{\text{ Err}} = 2.84 \) resulted in Fig. 11. In addition, the computational load \( t_e = 24 \text{ s} \) is smaller than \( t_e = 27.2 \text{ s} \) required in Fig. 10 and \( t_e = 53.5 \text{ s} \) required in Fig. 11.

![Figure 12](image-url)

Figure 12. Closed-loop operation of the reactor using the CLVNCP (FBTP, \( Ncol_{\text{max}} = 3; \ Ncol = 4 \text{ hr} \); \( N_{\text{steps}} = 3 \); \( N_{\text{ meas}} = 5 \); \( \text{DIST.} = -65\% \)).

Now, we take \( Ncol_{\text{max}} = 4 \) (\( N_{\text{steps}} = 4 \)) and repeat the above experiment. Fig. 13 shows the resulting output and input profiles. From this figure the values for \( C_i(t_b) = 0.604, C_i(t_b) = 0.072, T(t_b) = 314.8, I_{\text{ Err}} = 0.73 \) and \( t_e = 50 \text{ s} \). The performance improvement when compared against the previous run is achieved at the expense of an increase in the computational load.

Employing the optimization CLVNCP, two more experiments are carried out with \( Ncol_{\text{max}} = 5 \) and 6 (the corresponding \( N_{\text{ steps}} = 3 \) and 2, respectively). A summary of the results of the four experiments performed in this subsection is given in Table IV. It can be seen that a reduction in \( I_{\text{ Err}} \) is achieved at the expense of an increase in the computational effort. However, unlike the

<table>
<thead>
<tr>
<th>OR</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
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<td>2.923</td>
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<td>3.775</td>
<td>3.562</td>
<td>3.361</td>
<td>3.172</td>
<td>2.993</td>
<td>2.677</td>
<td>2.394</td>
<td>2.141</td>
<td>1.915</td>
<td>1.436</td>
<td>1.077</td>
<td>0.808</td>
</tr>
<tr>
<td>Ncol</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>1</td>
</tr>
</tbody>
</table>

TABLE III. OVERALL OPTIMIZATION PROCESS SHOWN IN FIG. 12 (Ncol_{\text{max}} = 3; \ Ncol = 4 \text{ hr} \); \( N_{\text{steps}} = 3 \); \( N_{\text{ meas}} = 5 \); \( \text{DIST.} = -65\% \))
results obtained for the CLVNFE, the concentration of the desired product increases as $N_{\text{col,\text{max}}}$ is increased. For comparable computational loads: (i) $I_{\text{Err}}$ has a lower magnitude in the CLVNCP than the corresponding value in the CLVNFE; and (ii) the desired product concentration in the CLVNCP is higher than the product concentration in the CLVNFE.

In all the online experiments, explained in the current subsection, the FBTP trial is assumed. Similar procedures can be carried out for the system if the MBTP testing is required.

In all the online experiments, explained in the current subsection, the FBTP trial is assumed. Similar procedures can be carried out for the system if the MBTP testing is required.

Table IV: CLVNCP ($n_i = 2; \tau_a = 4 \; h; \text{DIST.} = -65\%$)

<table>
<thead>
<tr>
<th>$N_{\text{col,\text{max}}}$</th>
<th>$N_{\text{steps}}$</th>
<th>$N_{\text{meas}}$</th>
<th>$\tau_d$ (h)</th>
<th>$C_a(t_0)$</th>
<th>$C_b(t_0)$</th>
<th>$T(t_0)$ (K)</th>
<th>$t_s$ (s)</th>
<th>$I_{\text{Err}}$</th>
<th>Fig.</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>5</td>
<td>12</td>
<td>1.002</td>
<td>0.071</td>
<td>314.3</td>
<td>24</td>
<td>0.76</td>
<td>12</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>20</td>
<td>0.804</td>
<td>0.072</td>
<td>314.8</td>
<td>50</td>
<td>0.73</td>
<td>15</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>3</td>
<td>28</td>
<td>0.609</td>
<td>0.074</td>
<td>316.6</td>
<td>92</td>
<td>0.67</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>38</td>
<td>0.571</td>
<td>0.081</td>
<td>318.5</td>
<td>274</td>
<td>0.34</td>
<td>-</td>
<td></td>
</tr>
</tbody>
</table>

VII. CONCLUSIONS

An appropriate input wave shaping combined with simultaneous optimization method improved the system operation when the batch reactor is operated in open loop. In the closed-loop operation, the online optimization CLVNCP developed in this article when compared against the CLVNFE: (i) imposes a lower computational effort to achieve comparable levels of $I_{\text{Err}}$ in the two methods; (ii) produces a higher level of the desired product concentration for comparable levels of the path violation errors $I_{\text{Err}}$ in the two methods; and (iii) increases the level of the desired product concentration as the optimization parameters are adjusted to reduce $I_{\text{Err}}$. This action reduces the product yield in the CLVNFE.

NOMENCLATURE

- $A_i$ inside heat-exchange area ($m^2$)
- $A_o$ outside heat-exchange area ($m^2$)
- $C_i$ concentration ratio of the component $i$ (kmol m$^{-3}$)
- $C_r$ specific heat of reactant ($J kg^{-1} K^{-1}$)
- $C_{pm}$ specific heat of metal ($J kg^{-1} K^{-1}$)
- $C_{pj}$ specific heat of cooling liquid ($J kg^{-1} K^{-1}$)
- $CH$ control horizon
- $DAE$ differential-algebraic equation
- $E_i$ activation energy for reaction $i$ ($J kmol^{-1}$)
- $FBTP$ fixed batch-time problem
- $F_i$ cooling liquid flow rate ($m^3 h^{-1}$)
- $I_{\text{Err}}$ integral of path violation error
- $A_{H_i}$ enthalpy of reaction for reaction $i$ ($J kmol^{-1}$)
- $k_0$ pre-exponential constant ($h^{-1}$)
- $k_i$ reaction rate constant for reaction $i$ ($h^{-1}$)
- $MBTP$ minimum batch-time problem
- $CLVNCP$ closed-loop method based on the VNCP
- $CLVNFE$ closed-loop method based on the VNFE
- $n_i$ number of finite elements
- $N_{\text{col}}$ number of collocation points on $u$ and $x$
- $N_{n_{\text{ele}}}$ number of collocation points on each finite element of $u$
- $N_{n_{\text{ele}}}x$ number of collocation points on each finite element of $x$
- $NLP$ nonlinear problem
- $N_{\text{meas}}$ number of measurements
- $NMPC$ nonlinear model predictive control
- $N_{\text{steps}}$ number of steps of the staircase

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OR  optimization run
p  parameter vector
PH  prediction horizon
Qj  amount of heat transferred to cooling liquid (J h⁻¹)
Qk  amount of heat transferred to metal (J h⁻¹)
Qt  amount of heat generated by the reaction (J h⁻¹)
R  universal gas constant J kmol⁻¹ K⁻¹
SQP  successive quadratic programming
t  time (h)
tb  batch time (h)
tc  average collocation time (h)
td  duration of control waveform (h)
e  computational effort
tg  threshold time gap
to  optimal batch time (h)
T  temperature of reaction mixture (K)
Tc  temperature of cooling liquid (K)
Tm  temperature of reactor metal (K)
U  inside heat-transfer coefficient (J h⁻¹ K⁻¹ m⁻²)
Uo  outside heat-transfer coefficient (J h⁻¹ K⁻¹ m⁻²)
V  volume of reactor contents (m³)
Vm  volume of cooling liquid (m³)
Vo  volume of reactor metal (m³)
VF E  variable number of finite elements
VFNP  variable number of collocation points
x  vector of variables

Greek letters
ρm  density of metal (kg m⁻³)
ρl  density of cooling liquid (kg m⁻³)

REFERENCES