Optimal Batch Process Regulation using Self-optimizing Control, NCO tracking

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Abstract: Optimal operation of batch processes in the presence of uncertainty has been an area of significant research interest. The use of online measurements as a source of information offers scope to mitigate the effects of uncertainty and attain optimal operation. Therefore, amongst the different approaches proposed to address the uncertainty issues, measurement based optimization approaches have been shown to be eminently suited. Measurements have been broadly used in two approaches, viz. self optimizing control (SOC) and tracking of necessary conditions of optimality (NCO). In an earlier work for continuous processes by Jäschke and Skogestad [1], the relative complementary roles of NCO tracking and SOC were clearly highlighted in terms of their applicability in combating the effects of different scales of uncertainty and disturbances. For batch processes, the NCO tracking is found to be successful, the complementary role of SOC is largely un-explored. In this work, we extend the integrated approach of Jäschke and Skogestad [1] to batch processes by redefining the NCO and SOC layers. The proposed framework is evaluated using simulations involving a nonlinear batch polymerization of styrene.

Keywords: Constraint Tracking; Dynamic Optimization; Necessary Conditions of Optimality, Polymerization, Self Optimizing Control

1. INTRODUCTION

Batch processes hold an important position in the chemical industry, especially in the manufacturing of speciality chemicals, pharmaceutical products, and polymers. Optimal regulation and control of batch processes is essential to produce consistent quality product in the presence of different uncertainty sources and disturbances. Uncertainties in batch processes stem from a poor knowledge about the cause-effect relationships and their associated parameters, initial condition variability and relatively larger term impact of different unknown disturbances that affect the processes. Such uncertainties render the model based control policies to be sub-optimal ad necessitate approaches that promote / preserve the optimality. On the other hand, shorter disturbances have a relatively smaller impact on the optimality but nevertheless need to be rejected so that the batch evolves along the best known optimal trajectories.

Batch processes exhibit several peculiar features that are not seen in continuous processes. The most conspicuous of these is the finite time duration of these processes due to which there are reduced time frames for mitigating the impact of uncertainty and disturbances. In the past advanced predictive controllers including shrinking diminishing horizon controllers have been proposed to mitigate the effects of short term disturbances and uncertainty. However, these model based approaches require high model fidelity in view of the shorter and diminishing horizons. While such model based optimization approaches can be used in the presence of reliable models, an alternate approach called measurement based optimization [6], [7] is also receiving increasing research attention. Measurements associated with batch processes can be available either online during the batch run as well as offline in batch archives. Both these kinds of measurements can potentially be used to improve batch productivity in the presence of uncertainty and disturbances. Online measurements can be used during batch operation to perform the tasks of state estimation and model update. As well, they could be used directly or indirectly in closed loop control algorithms to regulate the batch along pre-defined trajectories. Thus, in most cases (i.e. with the exception of model update), the use of online measurements has been more towards addressing short term or within batch corrections. When the model is updated using measurements, the new model could potentially be used to redefine the batch trajectories during the batch run; however such computations are very intensive to perform online. An alternate approach to using online measurements as proposed in [6] is to use measurements to directly update the control law by meeting the necessary conditions of optimality (NCO). They show that the above task of achieving optimality by meeting the NCO requires that both path constraints and end point sensitivities are tracked and met / satisfied. They propose the concept of solution models as a basis to perform the task of NCO tracking and ensuring optimality using the measurements.

On the other hand, self optimizing control (SOC) [4] advocates an off-line approach to preserve (near) optimality
in the presence of disturbances. The central idea in SOC is to find that combination or function of the measurements that will exhibit the least sensitivity to disturbances. For continuous processes, Skogestad [4], Alstad et al.[2] have proposed different approaches to generate this combination of measurements with specified disturbance rejection properties.

As mentioned earlier, there is generally a separation of time scales in the relative impact of uncertainty and disturbances on the optimality of the batch. For continuous processes, this difference in timescales has been exploited by way of a hierarchical decomposition of the control tasks, so that local and short term disturbance are rejected at the lower levels and the slower disturbances are accommodated at the upper levels. In accordance with these time scales and the relative properties of NCO tracking and SOC, it has been shown by Jäschke and Skogestad [1] for continuous processes, that these layers can be used in a complementary fashion with the NCO tracking addressing issues related to longer term uncertainty and the SOC focusing on rejecting short term disturbances.

To illustrate the concepts discussed above, we used the batch polymerization of Styrene reaction model from [5] and using two different disturbance cases, we show that the SOC-NCO combination can be successfully applied to Batch polymerization processes and the combination gives better results than the NCO tracking alone.

2. OPTIMIZATION VIA NCO TRACKING

In this measurement based optimization approach, NCO tracking structure is derived from the off-line numerical optimization of a nominal model and the control policies are updated on-line to satisfy the necessary conditions of optimality.

2.1 Dynamic optimization

Consider the following dynamic optimization problem:

\[
\min_{u(t), t_f} \Phi(x(t_f), t_f)
\]

such that

\[
\dot{x} = f(x, u)
\]

\[
0 \geq h(x, u)
\]

\[
0 \geq e(x(t_f))
\]

with initial conditions \(x(t_0) = x_0\)

where \(x(t) \in \mathbb{R}^n\) denotes the vector of state variables with the initial conditions \(x_0\), \(u(t) \in \mathbb{R}^m\) is the input vector, \(t_f\) is the final time, \(h\) are the path constraints and \(e\) are the end point constraints. By using Pontryagin’s minimum principle [8] the above problem can be reformulated with the Hamiltonian function \(H(t)\) as:

\[
\min_{u(t), t_f} H(t) = \lambda^T f(x, u) + \mu^T h(x, u)
\]

such that

\[
\dot{x} = f(x, u)
\]

\[
x(t_0) = x_0
\]

\[
\lambda^T = -\partial H/\partial x
\]

Here \(\lambda(t) \neq 0\) denotes the adjoint variables, \(\mu(t) \geq 0\) and \(\nu \geq 0\) the Lagrange multipliers for path and end-point constraints, respectively. A Lagrange multiplier is positive if corresponding constraint is active and zero otherwise. The NCO for the problem are shown in tabular form below:

<table>
<thead>
<tr>
<th>Type</th>
<th>Path Objectives</th>
<th>Terminal Objectives</th>
</tr>
</thead>
<tbody>
<tr>
<td>Constraints</td>
<td>(\mu^T h = 0)</td>
<td>(\nu^T e = 0)</td>
</tr>
<tr>
<td>Sensitivities</td>
<td>(\partial H/\partial u = 0)</td>
<td>(H(t_f) + \partial \Phi/\partial t_f = 0)</td>
</tr>
</tbody>
</table>

2.2 NCO tracking using a solution model

The four different objectives as given in the table above are satisfied by adjusting the manipulated variables through a decentralized control scheme. A solution model is then chosen to parametrize the inputs using time functions and scalars and then satisfying the different conditions through the model. The two major steps of the model are:

(1) Input Dissection: The inputs obtained after the numerical optimization step are divided into different arcs and the control switching structure is decided through the number and sequence of the input arcs. The input arcs are parametrized taking into account the active constraints. The time interval during which the input arcs are at their bounds are applied open loop since, these arcs are not affected by the presence of uncertainty. In other intervals, where the uncertainty affect the inputs, constitute the decision variables for the optimization problem.

(2) Linking the decision variables to NCO: After identifying the correct set of active constraints which does not change with uncertainty, the active constraints are linked with time functions if they belong to the set of path constraints. The active terminal constraints are linked with either scalar parameters or with time functions. Path and terminal sensitivities are met through the remaining degrees of freedom.

3. SELF OPTIMIZING CONTROL (SOC)

According to Skogestad [4], self-optimizing control is when one can achieve an acceptable loss with constant setpoint values for the controlled variables, without the need to reoptimize when new disturbances perturb the plant.

3.1 Null Space Method

The choice of control variables is key to overall performance of the control strategy. The null space method [3] is used to find the linear combinations of the measurements available to yield locally optimal control variables. Though, the preferred choice is to use single measurement specially if the loss is acceptably small, but in some cases the self-optimizing single measurement does not exist or is not available and the better choice left is to use measurement combinations.
In constrained optimization problem, some of the inputs are consumed in controlling the active constraints (with an assumption that the active constraints set does not change with time) and the remaining inputs are utilized to minimize the objective (cost) function \( J \) and therefore, the constrained problem can be seen as an unconstrained optimization problem with only remaining inputs to be used. If \( c \) is the linear combination of measurements \( y \), then

\[
c = Hy,
\]

where \( H \) is the constant measurement selection matrix. Alstad and Skogestad [3] have proved that with independent controlled variables \( c \) and no implementation error, a constant setpoint policy is optimal if the measurement combination \( c \) is independent of the disturbances \( d \) and hence, results in minimal loss to the optimal cost \( J \). It was shown by them that the measurement selection matrix \( H \) must lie in the left null space of the sensitivity matrix \( F \), given by:

\[
F = \frac{\partial y^{opt}}{\partial d}
\]

For the optimal measurement combinations to be independent of disturbances, \( H \) must satisfy the following condition:

\[
HF = 0
\]

4. COMBINING THE TWO TECHNIQUES: NCO TRACKING AND SOC

Jäschke and Skogestad [1] have proposed a way to combine the two techniques by using them in different layers of the overall plant control structure. The different layers of the control structure of a chemical plant are:

1. **Real Time Optimization (RTO):** This layer updates the setpoint values for the layer below at specified sample time. The infrequent updates make it necessary to pass the RTO output to a dynamic control layer below. NCO approach can be placed in this layer.

2. **Dynamic control layer:** Self-optimizing control can be placed in this layer. The SOC takes measurements form the plant and update the inputs so as to keep them at the setpoints provided by the RTO layer above it.

The null space method in SOC structure fails for the unexpected disturbances. The SOC structure, for cases in which the known disturbances take it far away from linearization point, fails. NCO tracking, on the other hand, is independent of disturbance knowledge. But in case of known disturbances which do not move the system too far from the optimal point the SOC gives faster response and the updates can be continuous or at relatively shorter sample times unlike the NCO procedure.

The above arguments suggest that the two techniques can actually be seen as complementary. When system encounters a known disturbance, SOC compensates for it without the need for reoptimization and larger or unknown disturbances can be handled with NCO tracking. The complementary structure also allows the NCO tracking to give better performance at reduced sampling time. Schematically, it can be represented as shown in Figure 1.

5. OPTIMIZATION OF POLYSTYRENE BATCH POLYMERIZATION

5.1 Process Description

The schematic diagram of the reactor [5] is shown in the figure 2. A 2-L jacketed reactor is used to carry out the reaction. The mixture of the styrene(70%) and toluene(30%) with initiator is placed inside the reactor with a stirrer to ensure proper mixing. A heater is used to provide the heat input and the reaction temperature is controlled with the help of the coolant flowing continuously through the jacket of the reactor. The coolant used is water at 294K and is moved continuously with the help of a peristaltic pump.

5.2 Problem Formulation

We have used the mathematical model of batch polymerization of Styrene given in [5] and it is not being presented here for brevity. The objective is to minimize the time required to reach 50% \( (X_{f_d}) \) conversion and 500 \( (X_{nf_d}) \) number average chain length such that the bounds on various variables are satisfied. The problem can be expressed mathematically as follows:

\[
\min_{Q,M,c,t_f} t_f
\]
For the heat input problem. The resulting solution is
inputs) to the NCO of the corresponding optimization
ables (the various intervals and switching times of the
A solution model is derived by linking the decision vari-
5.4 Solution Model
A solution model is derived by linking the decision vari-
escribed: 

\begin{align}
T_{min} &\leq T(t) \leq T_{max} \\
T_{j_{min}} &\leq T_{j}(t) \\
X(t_f) &\geq X_{f_d} \\
X_n(t_f) &\geq X_{n_{f_d}} 
\end{align}

Where reactor temperature \( T_{min} = 364K, T_{max} = 410K \) and jacket temperature \( T_{j_{min}}, T_{j_{min}} = 294K \).
The bounds on the inputs \( Q \) (heat input) and \( M_e \) (water input) are:

\begin{align}
Q_{min} &\leq Q(t) \leq Q_{max} \\
M_{e_{min}} &\leq M_e(t) \leq M_{e_{max}} 
\end{align}

where \( Q_{min} = 0W, Q_{max} = 170W, M_{e_{min}} = 0kg/s, M_{e_{max}} = 0.41 \times 10^{-3}kg/s \).

To evaluate the minimum final time \( t_f \), TOMLAB is used and the optimal profiles are obtained as shown in figures 3 to 6

The interpretation of the solution for each arc is as follows:
1. The heat input is at its maximum in the first arc and the water flow-rate at its minimum, the objective is to reach the optimal temperature range (374-394K) in which the monomer conversion is the fastest as early as possible.
2. The second arc of heat input ensures that the optimal temperature range is maintained at a constant rate of increase and the water flow-rate also aids in maintaining the optimal range of reactor temperature by reaching its maximum and thus, absorbing the extra heat generated but as soon as the the reactor temperature acquires a constant rate of increase, the water flow-rate again reaches its minimum.
3. Finally, while moving on the second arc, the heat input reaches its maximum value (arc 3) and is maintained at the level till the end of the process.

5.4 Solution Model
A solution model is derived by linking the decision variables (the various intervals and switching times of the inputs) to the NCO of the corresponding optimization problem. The resulting solution is
For the heat input \( U_1 \),

\begin{align}
arc1 : U_1 = U_{1_{max}} \text{ for } 0 \leq t < t_1 \\
arc2 : U_1 = K_n(y_{2_{opt}} - y_2(t)) \text{ for } t_1 \leq t < t_2 \\
arc3 : U_1 = U_{1_{max}} \text{ for } t_2 \leq t \leq t_f
\end{align}

where, \( y_2 = \frac{dT}{dt} \), \( K_n \) is a PI controller

For the water flow-rate \( U_2 \),

\begin{align}
arc1 : U_2 = U_{2_{min}} \text{ for } 0 \leq t < t_1 \\
arc2 : U_2 = U_{2_{max}} \text{ for } t_1 \leq t < t_2' \\
arc3 : U_2 = U_{2_{min}} \text{ for } t_2' \leq t \leq t_f
\end{align}

The switching time \( t_1 \) at which, both the inputs, the heat input and the jacket water flow-rate switch to their respective second arcs is determined when the reactor temperature reaches its optimum value (beyond which the reactor temperature not only moves away from the optimal temperature range but also eventually leads to reaction runaway). This is shown in the Figure 7
The switching time \( t_2' \) is determined when the heat input reaches its maximum while moving on arc2 and the switching time \( t_2' \) is determined when the reactor temperature reaches a constant rate of increase while the arc2 of heat
6. SELF OPTIMIZING CONTROL(SOC) FOR A DYNAMIC PROCESS

Once again citing the Skogestad’s definition of SOC [4], Self-optimizing control is when we can achieve an acceptable loss with ‘constant’ setpoint values for the controlled variables without the need to reoptimize when disturbances occur.

Skogestad in the same paper also suggests that for the unsteady-state processes setpoints can be precomputed trajectories as a function of time. Here, instead of computing a trajectory of setpoints, a single constant setpoint (despite being an unsteady-state process) is taken to effectively reject the known disturbances. The constant setpoint is computed using the Null Space method which is again suggested by Alstad and Skogestad [3] for steady-state processes only. The idea here is to find a (estimated) measurement which remains constant and changes only in the presence of disturbances. If we see the optimal profiles of reactor and jacket temperatures shown in the Figure 3, we find that the slopes of the reactor and jacket temperatures remain constant while the arc2 of heat input is applied to the process.

The constant setpoint is calculated for the combination of the two temperature slopes. For finding the constant setpoint value $C_s = H y$, sensitivity matrix F is to be computed first. Two cases of disturbance rejection are considered. Both cases are simulated on Simulink (MatLab):

Case1: Disturbance introduced is again the coolant temperature which is varied ±5K from its value of 294K. F is calculated using finite difference approximation:

$$F = \frac{1}{T_j^+ - T_j^-} (y^+ - y^-)$$  \hspace{1cm} (27)

Where $T_j^+ = 299K, T_j^- = 289K$, $y^+$ and $y^-$ correspond to the slopes of jacket temperature($y_1$) and reactor temperature($y_2$).

The value $f_1$ corresponding to change in slope of jacket temperature is equal to 0.119 and the value of $f_2$ corresponding to change in the slope of reactor temperature is 2.2. calculating the matrix H,

$$h_1 * 0.119 + h_2 * 2.2 = 0$$  \hspace{1cm} (28)

which gives $h_1 = 18.67$ when $h_2$ is taken as -1.

using these values and calculating the value of $C_s = h_1 y_1 + h_2 y_2$ gives,

$$C_s = 0.179$$  \hspace{1cm} (29)

After implementing the SOC with the help of a PID controller, the impact of change in water temperature to 299K on SOC-NCO and NCO alone is compared and is shown in the Figure 10. Figure 10 clearly depicts the effectiveness of using the SOC-NCO combination instead of using NCO alone. The SOC-NCO combination not only gives better conversion it also reaches the desired rate faster than NCO alone.

Case2: The sensitivity matrix $F$ is found for a different disturbance range of water temperature, in this case water temperature is disturbed from 294K to 284K. Using the
null-space method as used in the Case1, the value of $C_s$ comes out to be 5.07. Disturbance rejection capabilities of the two techniques is compared for a disturbance of -8K and again SOC-NCO outperforms NCO alone. The comparison is shown in Figure 12.

### Table

<table>
<thead>
<tr>
<th>Case</th>
<th>NCO Tracking</th>
<th>SOC-NCO</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case1</td>
<td>reaches asymptotically</td>
<td>7200 sec</td>
</tr>
<tr>
<td>Case2</td>
<td>7300 sec</td>
<td>6850 sec</td>
</tr>
</tbody>
</table>

The above table shows the time required to reach 50% conversion using different control techniques for disturbance rejection cases 1 and 2. In the disturbance case 1, NCO tracking reaches the conversion rate asymptotically, while the SOC-NCO combination take around 7200 seconds. For the second case, the SOC-NCO combination takes 450 seconds less to settle to the desired conversion.

### 7. CONCLUSION

An SOC-NCO combination is developed for the batch polymerization of Styrene and it has been found that the combination is much more powerful in rejecting ‘known’ disturbances then the NCO tracking alone while simultaneously meeting the objective of minimum time to conversion. As suggested by Jäschke and Skogestad [1], NCO can be placed in the upper control layer (RTO) and SOC in the lower dynamic control layer. SOC can reject known small disturbances and hence, the need to re-optimize each time a small known disturbance occurs, goes away. For bigger magnitude disturbances or unknown disturbances, NCO can update the SOC set-point. The SOC-NCO combination is applied successfully to batch polymerization process utilizing simple null space method.

### REFERENCES


