An investigation of Economics-Driven NMPC-Formulations for a Continuous Catalytic Distillation System

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Abstract: For continuously operated processes, even a small increase in the efficiency pays important dividends in terms of energy savings and profit. Therefore, tighter and more efficient control of chemical plants is becoming a strategic objective. In this work, we demonstrate the use of dynamic process optimization to improve the business performance of chemical processes. Model predictive control techniques are widely applied to coupled multivariable control problems. The reference values in these problems are usually adjusted by infrequent optimizations based upon a static rigorous nonlinear model of the plant. In between these optimizations, however, the process may undergo sub-optimality of operation due to the presence of disturbances. In this paper, nonlinear model-based optimization with different schemes is proposed to combine optimal operation and feedback control. The work demonstrates the feasibility and the potential of using optimizing as well as economics-oriented tracking control techniques for a challenging example, a catalytic distillation process. The performances of the proposed controllers are investigated and compared. This work points out that by using direct optimizing NMPC, the plant economics can be handled better while guaranteeing the product specifications.

Keywords: Online dynamic economic optimization, nonlinear model predictive control, continuous catalytic distillation, non-minimum phase behavior.

1. INTRODUCTION

Economics-driven optimization based on rigorous first-principles models has been increasingly integrated into the decision-making policies in the operation of chemical processes in order to improve the competitiveness of the processes. These decisions are usually made based on infrequent optimizations of stationary rigorous first-principles models. It has been recognized that the static nature of these models can lead to infeasibility issues and performance degradation. Using rigorous dynamic models in the decision-making policies gives the possibility to avoid these limitations, and therefore higher process efficiency and profitability can be achieved. This can be realized using different strategies of economics-based nonlinear model predictive control (NMPC) schemes (Engell(2007)), (Zavala and Biegler (2009)). For a historical view of the changing role of process control in operation and profit/loss measures besides the perspective of how process control has influenced business decision-making, see (Edgar (2004)). A general motivation on how model predictive control techniques and dynamic process optimization can be integrated to improve economic performance of chemical processes is given in (Backx et al. (2000)). In the work presented here, a complex dynamical model is used to optimize the operation of a continuous catalytic distillation process for the production of methyl acetate. Methyl acetate, also known as methyl ethanoate, is a carboxylate ester mainly used as a volatile low toxicity solvent for a broad range of coatings (e.g. paints), cosmetics and printing ink resins. It is also used as an intermediate in a variety of chemical synthesis applications.

The paper is organized such that the next section gives a short overview on NMPC and the mathematical formulation of different NMPC strategies. In section 3, a brief description of the catalytic distillation process, its mathematical modeling and the economic function used in this work are presented. Section 4 describes the structure of the control algorithm. In section 5 the performance of the NMPC strategies is discussed. The paper closes with conclusions in section 6.

2. NONLINEAR MODEL PREDICTIVE CONTROL

NMPC is an advanced feedback control technique the popularity of which comes mainly from its ability to handle constrained and MIMO systems and because general economic optimization criteria can be integrated into the feedback control design. The basic principle of NMPC is to select a set of future control actions or decision variables over a control horizon length of $M$ in order to minimize an objective function and to satisfy all the imposed constraints over a predefined prediction horizon $P$ using a nonlinear model. Fig. 1 demonstrates the idea behind NMPC. The objective function, which can be a tracking, a maximizing or an economic criterion, is
usually complemented by some linear and/or nonlinear constraints, besides the dynamic model itself. Although the optimization is performed over a control horizon $M$, only the first control action is actually implemented. Next, the plant output measurements are obtained and then a compensation of plant-model mismatch is carried out using a bias correction as the difference between the plant measured output $y_{meas}$ and the model output $y_{model}$ at the current time interval to adjust the output prediction. Then the optimization problem is solved again.

2.1 Mathematical formulation

Conventional Tracking Control (CTC) The conventional tracking objective is the squared sum of the differences between the predicted outputs and the setpoints over the prediction horizon. A slew rate term is added to the objective index to penalize excessive control actions and to smoothen the response. The mathematical formulation of the tracking controller is as follows:

$$\min_{\Delta u_1(1), \ldots, \Delta u_1(k + M), \ldots, \Delta u_k(1), \ldots, \Delta u_k(k + M)} \Phi_{CTC}(x, u)$$

subject to:

$$x_{i+1} = f(x_i, \vartheta_i, u_i, i), \ i = k, \ldots, k + P$$

$$u_{min} \leq u(i) \leq u_{max}, \ i = k, \ldots, k + M$$

$$-\Delta u_{min} \leq \Delta u(i) \leq \Delta u_{max}, \ i = k, \ldots, k + M$$

where $x_i$ refers to the differential state variables while $\vartheta_i$ denotes algebraic variables. $f$ represents the system dynamics. $\alpha$ and $\gamma$ are the weights on the control inputs and the outputs respectively. $y_{n, ref}$ refers to the setpoint or the desired output trajectory, $y_n$ is the corrected model prediction. $N$ is the number of the controlled outputs, $R$ is the number of the control inputs. Compensation for the plant-model mismatch is done using the following bias correction equations:

$$d_n(k) = y_n^{meas}(t(k)) - y_n^{model}(t(k)),$$

$$\hat{y}_n(k + i) = y_n^{model}(k + i) + d_n(k), \ i = 1, \ldots, P.$$

Where $d_n$ denotes the current difference between the plant and the model, $\hat{y}_n$ is the corrected model predictions (Fernholz and Engell (2000)).

Moving Horizon Optimizing Control (MHOC) In the optimizing controller, the feedback control and the optimal operation of the plant are integrated. An economic cost criterion replaces the conventional quadratic criterion that penalizes the deviations of the controlled variables from the reference values and the input variations. Product quality specifications as well as process limitations are included in the optimization problem as constraints. An important point in favor of using an economic cost criterion and formulating restrictions of the process and the product properties as constraints is that this reduces the need for tuning of the weights in less explicit formulations. This approach has a number of further advantages (Engell (2007)):

- Immediate reaction to disturbances, no waiting for the plant to reach a steady state is required.
- The exact constraints can be implemented for measured variables and only the model error has to be taken into account for unmeasured constrained variables, so the "safety band" can be reduced.
- Over-regulation is avoided, no variables are forced to fixed setpoints and all degrees of freedom can be used to improve the economic performance of the plant as shown e.g. in (Idris and Engell (2011)).
- No inconsistency arises from the use of different models on different layers.
- Economic goals and process constraints do not have to be mapped to a control cost whereby economic optimality is lost and tuning is difficult.

The overall scheme is structurally simple.

The general mathematical formulation of the direct online optimizing control is shown below:

$$\min_{\Delta u_1(1), \ldots, \Delta u_1(k + M), \ldots, \Delta u_k(1), \ldots, \Delta u_k(k + M)} \Phi_{MHOC}(x, u)$$

subject to:

$$x_{i+1} = f(x_i, \vartheta_i, u_i, i), \ i = k, \ldots, k + P$$

$$u_{min} \leq u(i) \leq u_{max}, \ i = k, \ldots, k + M$$

$$-\Delta u_{min} \leq \Delta u(i) \leq \Delta u_{max}, \ i = k, \ldots, k + M$$

$$u(i) = u(k + M), \ \forall i > k + M$$

Where $\beta_i$ are the weights on the bias correction equations.

$$\sum_{i=1}^{P} y_{i, k+i} \leq L_{y_i}.$$
describes how much effort the controller should invest to maximize the profitability/productivity or to which extent it is permitted for the process to deviate from the setpoints. This parameter must be carefully chosen using intensive simulations since a larger value of this parameter can lead to higher profit but off-specifications products.

3. CONTINUOUS CATALYTIC DISTILLATION

3.1 Process description

Catalytic distillation (CD) has economical and environmental advantages over a reaction step followed by conventional distillation steps. For systems with appropriate chemistry and vapor-liquid phase equilibrium, catalytic distillation combines the reaction and the separation operations, which reduces energy demand, capital costs and environmental impact. This process is particularly suitable for esterification reactions since the main obstacle in most of these reactions is the unfavourable chemical equilibrium which limits conversion. This obstacle can be overcome e.g. by a large excess of one of the reactants, or more preferably by the removal of reaction products according to Le-Chatelier’s principle.

Compared with other integrated reaction and separation processes, catalytic distillation (heterogeneously catalyzed reactive distillation) represents one of the most important applications of the concept of process intensification and it has numerous application in the petrochemical industries (Richter, Górák and Kenig (2006)). Using CD columns, the conversion can be increased beyond the equilibrium due to the continuous removal of reaction products from the reactive zone. This also helps in overcoming potential azeotropes and improves energy integration. Enhanced reaction selectivity is also one of the advantages of CD columns (Noeres, Kenig and Górák, 2003). In the showcase example of the methyl acetate production process of Eastman of Chemicals, a plant consisting of two reactors and eight distillation column was replaced by a single reactive distillation column (Asgede, Partin and Heise (1990)). Since different functionalities are implemented into one reactive separation process, complex dynamics in the catalytic area that result from the integration of reaction and separation and the reduced number of degrees of freedom due to the identical temperatures and pressures can be considered as significant challenges of these processes.

The physical unit consists of three main parts: the condenser, the packed column, and the reboiler, see Fig. 2. The packed column comprises four sections: one enriching packing in the top, two catalytic packings in the middle in which the chemical reaction takes place, and a stripping packing in the bottom. The system has four inputs which can be adapted in order to achieve the desired products specifications. These inputs are the reboiler heat duty, the condenser reflux ratio and the flow rates of the two reactants.

3.2 Dynamic model of the CD column

In general, there are two different types of dynamic models that have been employed for catalytic distillation: the
equilibrium model and the rate-based (non-equilibrium) model. For a detailed comparison study between these different models for packed catalytic columns, see (Peng, Edgar and Eldridge (2003)). In this work, the catalytic distillation column is described by an equilibrium stage model where it is assumed that the vapour and the liquid stream leaving each stage are in thermodynamic equilibrium with each other. The core of the model are the MESH equations, consisting of the material balance equations, the phase equilibrium relations and the summation equations or the constitutive relations of the liquid and vapour mole fractions. \( H \) stands for the heat or the enthalpies of the liquid and/or the vapour phases (Taylor and Krishna (2000)).

The equilibrium stage model is extended by additional equations for the reaction kinetics and the dynamics of the tray hydraulics. For a detailed description of the dynamic model and the modelling assumptions, see (Kreul and Górák (1998)). Modelling results in a large differential algebraic system (DAEs) with nearly 600 states in which the dynamics of the process are described by 90 differential states, the rest being algebraic variables.

The model that is used inside the controller for online optimization has been slightly simplified, by this simplification about 12% of the states (most of them being algebraic variables) are removed and the computation time is reduced by about 30%. The simplified model still captures most of the dynamics of the equilibrium-based stage model correctly, for a comparison between the full model and the reduced one we refer to (Idris and Engell (2011)).

### 3.3 Control structure

Besides the high nonlinearity of the model, the process exhibits non-minimum phase behaviour (inverse response) as illustrated in Fig. 3. The system also shows a change of the sign of the static gain (input multiplicities) in all input channels. In Idris and Engell (2011), it was proposed to use a MIMO-control structure for this process considering the reflux ratio, heat supplied to the reboiler and the feed flow rates of the reactants as the manipulated variables, while the concentrations of MeAc in the distillate and the conversion of the MeOH are the controlled variables. In this work, all the inputs mentioned above except the heat duty are exploited as control degrees of freedom while the concentration of \( \text{H}_2\text{O} \) in the bottom stream is used as a controlled variable instead of the conversion of MeOH.

The purity of the side-product (water) in the bottom represents an indirect measure of the conversion inside the column. The top product purity is defined mathematically as:

\[
\text{Purity}_{\text{MeAc},k+1} = \frac{D_{\text{MeAc},k+1}}{D_{T,k+1}},
\]

while the purity of the water in the bottom is defined as:

\[
\text{Purity}_{\text{H}_2\text{O},k+1} = \frac{B_{\text{H}_2\text{O},k+1}}{B_{T,k+1}},
\]

where \( D_{\text{MeAc},k+1} \) is the number of moles of the MeAc in the distillate at time \([k + 1]\), \( D_{T,k+1} \) is the total number of moles in the distillate at time \([k + 1]\), \( B_{\text{H}_2\text{O},k+1} \) is the number of moles of \( \text{H}_2\text{O} \) in the bottom at the time \([k + 1]\), \( B_{T,k+1} \) is the total number of moles in the bottom at time \([k + 1]\). The reactant feeds are considered to be pure components. The formulation of the economical function considered here is as follows:

\[
\Psi = \{\text{Product revenue} - \text{energy cost} - \text{cost of feeds}\},
\]

which can be rewritten mathematically as:

\[
\Psi(k) = \left( \hat{P}(k)C_P - H(k)C_E - \sum_{j=1}^{N_f} \hat{R}_j(k)C_{R,j} \right),
\]

where \( \Psi(k) \) is the profit function value at time \([k]\), \( N_f \) is the number of feed streams, \( \hat{P}(k) \) is the product flow rate at time \([k]\), \( C_P \) is the product unit price, \( H(k) \) is the boil-up rate at time \([k]\), \( C_E \) is the price per energy unit, \( \hat{R}_j(k) \) are the feed flow rates at time \([k]\), \( C_{R,j} \) are the unit prices of the feeds.

### 4. STRUCTURE OF THE CONTROL ALGORITHM

The control algorithm illustrated in Fig. 4 was implemented in gPROMS, using MATLAB and TOMLAB (see TOMLAB User’s Guide (2010)). The Excel spreadsheet server is used to update the initial conditions and the control inputs at each iteration. The differential-algebraic equations of the optimization model and the plant model are integrated using gPROMS’ DAE solver “DA SOLV”, while the optimization is conducted in the TOMLAB optimization environment using the “SNOPT” NLP solver.

The objective function and the constraints are implemented in MATLAB which also performs data management and some coordinating tasks such as calling the gPROMS simulation, extracting and exchanging the required data among different modeling platforms as well as...
Fig. 4. The designed control algorithm.

updating the initial conditions in the Excel spreadsheet. After the simulation of the full and the reduced models with the newly obtained optimal inputs, a compensation of the plant-model mismatch is done by adding the differences to the predicted outputs in the cases of the pure tracking and economics-oriented tracking control and to the purity constraints in the case of the optimizing control. The initial conditions of the optimization model are updated by the current states of the plant model which are assumed to be ideally estimated and then the optimization is performed again. The effect of the state estimator on the control performance will be considered in further studies.

The routine SNOPT is a general-purpose algorithm. It is suitable for large-scale constrained optimization. It minimizes a linear or nonlinear function subject to bounds on the variables and sparse linear or nonlinear constraints. SNOPT applies a sparse sequential quadratic programming (SQP) method using limited-memory quasi-Newton approximations to the Hessian of the Lagrangian. The merit function for step length control is an augmented Lagrangian. It requires less matrix computations and fewer evaluations of the functions than its counterpart solvers (e.g. NPSOL and MINOS) and it is efficient if many constraints and bounds are active at a solution (Murray, Gill and Saunders (2002)).

5. CONTROL PERFORMANCE AND DISCUSSION

The results show that three different operating points exist; each controller has converged to a different operating point. The operating points chosen by the economics-oriented tracking controller and the optimizing control has led to almost same profit. These multiple solutions may lead to numerical problems, e.g. slower convergence to the optimal solution and computational delay. All controllers were able to react according to the intended goals. The economics-oriented tracking controller manages to track the purity references while improving the economics of the process. The optimizing controller on the other hand is able to satisfy the product purity constraint and over-purifies the water in the bottom while maximizing the economical revenue of the plant. The parameters of both controllers are shown in Table 1 below. Comparing the performance of all controllers, the tracking NMPC controller moves to the setpoints in directions that are not the best for process economics, while the moving horizon optimizing NMPC controller satisfies the constraints first and then moves towards the maximally profitable operation. A higher water purity at the bottom stream is more favorable for a higher profit. The moving horizon optimizing controller outperforms the economics-oriented tracking controller and achieves about 8.22 % improvement in the profit over the conventional tracking NMPC’s profit, while the economics-oriented tracking controller obtains about 6.96 % higher profit than that of the conventional tracking controller. It can be observed that the profit

<table>
<thead>
<tr>
<th>Controller</th>
<th>CTC, EoTC and MHOC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Prediction horizon, P</td>
<td>3.5-3.9 min.</td>
</tr>
<tr>
<td>Control horizon, M</td>
<td>1</td>
</tr>
<tr>
<td>Regularization, α</td>
<td>0.0001, 0.001, 0.001</td>
</tr>
<tr>
<td>Sampling time, h</td>
<td>5 min.</td>
</tr>
<tr>
<td>Plant order</td>
<td>581</td>
</tr>
<tr>
<td>Model order</td>
<td>511</td>
</tr>
<tr>
<td>Output weights, γ</td>
<td>12</td>
</tr>
<tr>
<td>Economics weights, β</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 1. The parameters of the controllers.
control, however, the response slightly violates the product specifications and exhibits a control offset. Fig. 6 shows the evolution of the relative magnitude of the economics to the tracking terms in the objective function of the EoTC controller. The average computation times of all controllers are shown in Table 2. The computation times of the optimizing controller are much longer compared to the tracking-based controllers. Compared to the use of the "glc-Solve - DIRECT" algorithm in our previous work, the computation times of the optimizing controller are considerably higher which was not expected. Many function evaluations are needed because of the non-quadratic objective function. Tuning of the optimizer settings (e.g., restricting the number of major and minor iterations, and setting the tolerances of the objective function and the constraints) to speed up the computation times led to a deteriorated response and to a suboptimal economic performance. It is worth to note here that, the SNOPT optimization solver was able to produce smooth responses for all controllers despite of the model errors and the assumed measurement and actuator noise.

6. CONCLUSION AND FUTURE WORK

The optimizing and the economics-oriented tracking controllers have been applied successfully to a simulated complex model of a catalytic distillation column with plant-model mismatch. By optimizing nonlinear control, the plant economics can be enhanced without sacrificing product specifications. The economics-oriented tracking controller can also improve the plant economics when more degrees of freedom than controller variables are present, however, it can also lead to off-specifications product and therefore intensive parameter tuning studies are needed. The application of the optimizing control approach to industrial chemical plants still requires more efficient optimization solvers and simulation tools for guaranteed real-time capability. Different control structures as well as the effect of a state estimator on the performance of the controllers will be studied in future work.

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