Proceedings of the 17th World Congress
The International Federation of Automatic Control
Seoul, Korea, July 6-11, 2008

Nonlinear model predictive control of an industrial batch reactor subject to swelling constraint

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Abstract: This paper presents the application of nonlinear model predictive control (NMPC) to a simulated industrial batch reactor subject to safety and productivity constraints due to swelling. The catalyst used in the chemical process decomposes in the reactor; therefore it is fed in discrete time steps during the batch. Although the optimal reactor temperature profile, using a fixed catalyst dosing policy, is optimized off-line an on-line control solution is needed in order to accommodate the reaction rate and level disturbances which arise due to catalyst dosing uncertainty (feeding time and mass). The on-line control method is based on the shrinking horizon optimal control methodology and it uses a reaction and hydrodynamic model. It is concluded that the implemented shrinking horizon on-line optimization strategy is able to calculate the optimal temperature profile without causing level swelling.

1. INTRODUCTION

Since the advent of dynamic matrix control (DMC), model predictive control (MPC) has been the most popular advanced control strategy in the chemical industries (Morari and Lee, 1997). Linear MPC has been heralded as a major advance in industrial control (Richalet et al., 1978). However, due to their nonstationary and highly nonlinear nature, linear model based control usually cannot provide satisfactory performance in the case of complex batch processes (Qin and Badgwell, 2003). Nonlinear model predictive control (NMPC) reformulates the MPC problem based on nonlinear process models, providing the advantage to cope inherently with process nonlinearities (Allgower et al., 2004) characteristic to batch systems including robust formulations (Nagy and Braatz, 2003). The presented paper illustrates the benefits of an efficient on-line optimizing non-linear model based control to a simulated industrial batch reactor subject to the level constraint from safety and productivity considerations which arise from the industrially relevant problem of potential swelling.

Reactor content swelling occurs when the vessel content level rises due to a gas or vapor stream that passes through the liquid. The vapor or gas stream can have different sources: gas is injected in liquid phase reactors where a reaction has to be carried out; vapor flow occurs in a reactor when the reaction produces a gas phase product which travels to the reaction mass surface; another reactor level rise is due to direct steam heating when some of the steam does not condense and disengages to the top of the vessel. As a result of the swelling phenomena reaction mass enters the pipes and the condensers connected to the reactor. As a consequence of such undesired events reactor shut-down is mandatory and production time is lost for cleaning operations. The pipe and condenser cleaning is carried out by charging solvent which is evaporated and condensed for a certain time (refluxing conditions). Reactor or evaporator content swelling phenomena can lead to significant productivity losses if it is not considered during process operation and is regarded as a reactor productivity and safety problem; the off-line optimal temperature control of batch reactors with regard to swelling was subject of investigation (Simon et al., 2008). This work aims to implement a model based level control strategy, which considers reaction content swelling. The on-line strategy is required to accommodate the reaction rate disturbances which arise due to catalyst dosing uncertainties (catalyst mass and feed time).

2. DYNAMIC MODELLING OF THE INDUSTRIAL BATCH REACTOR SWELLING

The system considered in this study is based on a proprietary industrial batch process, for which the model has been developed and identified. The catalyst used in the chemical reaction decomposes in the reaction mixture; therefore it is fed several times during the process operation. The first feeding takes place at the beginning of the operation, later on the catalyst shots are added as the reaction rate decreases. This type of process operation is often used in the industrial practice. The process is characterized by significant uncertainties in the kinetic constants and in the addition time of the catalyst. Figure 1 shows the experimental reaction rate measurements (normalized data) from the real industrial plant, in the case of repeated application of the same recipe with two consecutive catalyst dosings. The significant bath-to-batch variation of the reaction rate can be observed, which can be countered by the design of suitable control.

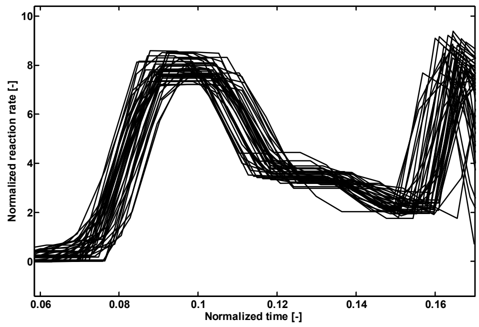

Fig. 1 Change of the reaction rate in time for the industrial batch process.

The reactor level is controlled using the temperature as the manipulated variable in order to compensate for the change in the reaction rate. The process operation can be optimized off-line by calculating an optimal temperature profile in function of the catalyst dosage time, dosed mass and purity. However the off-line calculated optimal temperature profile does not ensure safe operation in the case of disturbances in the catalyst feeding policy. Hence an on-line control strategy is needed to recalculate the temperature profile during the operation considering the unknown disturbances. The on-line control strategy used here is based on the nonlinear model predictive framework. During the beginning of the process operation, until the complete dissolution of component A, (1), the reactor system consists of three phases: solid, liquid and gas. Four equilibrium reactions in series take place in the liquid phase and a catalyst is used in solubilized form. The reaction scheme is as follows:

$$A_s \rightleftarrows A_l \tag{1}$$
$$A_l + B \rightarrow C + D \tag{2}$$
$$B + C \rightarrow E + D \tag{3}$$
$$B + E \rightarrow F + D \tag{4}$$
$$B + F \rightarrow P + D \tag{5}$$

where A_s and A_l represent component A in solid and liquid phase, respectively. Raw materials are components A and B; components C, E, F are intermediates and P is the desired product. Product D is in vapor phase at the temperature and pressure conditions in the reactor, and the production of the co-product D creates a vapor flow that travels to the reaction mass surface and produces a certain void fraction in the liquid mass. The extent of the void fraction is dependent on the liquid properties and vapor hold-up in liquid phase which in turn are dependent on the vapor flow rate, thus on the reaction rate of gas product D.

The solid-liquid mass transfer was modeled based on the Noyes-Whitney equation (Noyes and Whitney, 1887) which is based on the assumption that the rate of dissolution of a solid is dependent upon its solubility, its concentration driving force, its diffusivity, and the surface area of the solid:

$$\frac{dn_{As}}{dt} = \frac{-3}{1000}\left(n_{As0}MW_A\right)^{1/3}\left(n_{As}MW_A\right)^{2/3}\frac{k_{MT}}{\rho_A R_{P0}}\left(\frac{n_{Aliq}^{eq} - n_{Aliq}}{V}\right) \tag{6}$$

where n_{As0} (kmol) is the initial mole number of solid component A, n_{As} (kmol) is the mole number of solid component A at any time t, n_{Aliq} is the mole number of dissolved component A in liquid phase (kmol), MW_A is the molecular weight of component A (kg/kmol), ρ_A is the solid component A density (kg/m^3), R_{P0} is the initial solid component A pellet radius (m), k_{MT} (m/s) is the solid-liquid mass transfer coefficient (defined as the ratio of diffusivity and diffusion layer thickness) and n_{Aliq}^{eq} is the equilibrium solubility of component A in B (kmol). The solid particles are assumed to be mono-disperse spheres and the number of particles does not change in time. The most important phenomena which were not modeled are the non-ideal mixing, and the particle size distribution of solid component A.

The basic assumption of the kinetic model is that the reactions take place in liquid phase. In order to model the forward reactions the Arrhenius formulation is implemented, using a reference reaction constant determined at a reference temperature:

$$r_{R,i} = k_{ref,i}\exp\left\{-\frac{E_{A,i}}{R}\left(\frac{1}{T_r} - \frac{1}{T_{ref}}\right)\right\}\frac{n_{Cat}\, n_B\, n_X}{V^3} \tag{7}$$

where i is the ith reaction step, $r_{R,i}$ is the ith reaction rate to the right-hand side (kmol/m^3/s), $k_{ref,i}$ are the corresponding rate constants at reference temperature (m^6/kmol^2/s), $E_{A,i}$ the activation energies (kJ/kmol), T and T_{ref} are the current and reference temperature (K), R is the gas constant (kJ/kmol/K), n_{Cat} is the catalyst mass in the reactor (kmol), n_B is the mole number of component B (kmol), n_X represents the number of moles of component X, that is, n_{Aliq}, n_C, n_E and n_F (kmol), respectively, and V is the volume of the reaction mass (m^3). During the reaction the volume changes significantly, therefore V is a variable in the model. The reaction volume is not constant due to two factors: on one hand there is the removal of by-product D and on the other hand the density of the mixture changes. These two effects contribute each with about 10% volume change. The reaction volume at any time is calculated in function of the densities and masses of all components in the mixture thus accounting for the removal of co-product D and the change in composition. The resulting component mass balances for the liquid phase are as follows:

$$\frac{dn_{Aliq}}{dt} = -\frac{dn_{As}}{dt} - r_{R,1}V \tag{8}$$

$$\frac{dn_B}{dt} = \left(-r_{R,1} - r_{R,2} - r_{R,3} - r_{R,4}\right)V \tag{9}$$

$$\frac{dn_C}{dt} = \left(r_{R,1} - r_{R,2}\right)V \tag{10}$$

$$\frac{dn_E}{dt} = \left(r_{R,2} - r_{R,3}\right)V \tag{11}$$

$$\frac{dn_F}{dt} = (r_{R,3} - r_{R,4})V \tag{12}$$

$$\frac{dn_P}{dt} = r_{R,4}V \tag{13}$$

In order to describe the effect of liquid swelling the pool void fraction, is used. The swelled height H [m] in terms of the average pool void fraction $\bar{\alpha}$ and the height of the resting liquid H_0 [m] is given by (14):

$$H = \frac{H_0}{1-\bar{\alpha}} \tag{14}$$

The Churn turbulent hydrodynamic model was developed by the Design Institute for Emergency Relief Systems (Fisher et al., 1992). In this model it is considered that boiling takes place throughout the entire volume of liquid, rather than solely at the surface. Each bubble occupies volume and displaces the liquid surface upward. Individual bubbles are able to rise (slip) through the liquid with a velocity that depends on the buoyancy and surface tension and are retarded by viscosity and the foamy character of the fluid. The Churn turbulent vessel model assumes uniform vapor generation throughout the liquid with considerable vapor-liquid disengagement in the vessel. The degree of vapor-liquid disengagement is represented by the following relationship (Fisher et al., 1992):

$$\bar{\alpha} = \frac{j_g / U_\infty}{2 + C_0 (j_g / U_\infty)} \tag{15}$$

where j_g is the vapor superficial velocity (m/s), C_0 is a data-correlating or distribution parameter with values ranging from 1.0 to 1.5. The characteristic bubble rise velocity, U_∞ (m/s), for the Churn-turbulent model is given by the following expression:

$$U_\infty = \frac{20.0949 \cdot (4.5134 \cdot 10^{-4} \sigma g (\rho_f - \rho_g))^{0.25}}{\sqrt{\rho_f}} \tag{16}$$

where σ is the interfacial tension (kg/s^2), g is the acceleration due to gravity (m/s^2), ρ_f (kg/m^3) is the liquid density, and ρ_g (kg/m^3) is the vapor density.

The connection between the chemical reactor model (system of differential algebraic equations - DAE) and the hydrodynamic model (system of algebraic equations - AE) is made by the formation rate of co-product D $(dn_D / dt = -dn_B / dt)$ and the ideal gas law. The formation rate is converted into volumetric flow rate and by division with the reactor area is converted into gas velocity, j_g. Using the hydrodynamic model and the calculated gas velocity the swelled reactor level H is calculated.

3. ON-LINE OPTIMIZING CONTROL FOR SWELLING CONSTRAINED BATCH REACTOR

The model is represented as a generic ODE system:

$$\dot{x}(t) = f(x(t), u(t)) \tag{17}$$

$$y(t) = g(x(t), u(t)) \tag{18}$$

subject to the input, state and output constraints

$$u(t) \in \mathcal{U},\ x(t) \in \mathcal{X},\ y(t) \in \mathcal{Y} \tag{19}$$

where $x(t)$ is the n_x vector of states, $u(t)$ is the n_u set of input vector trajectories and $y(t)$ is the n_y vector of output variables. The sets $\mathcal{X}$ and $\mathcal{Y}$ are closed subsets of $\mathbb{R}^{n_x}$ and $\mathbb{R}^{n_y}$, respectively and the set $\mathcal{U}$ is a compact subset of $\mathbb{R}^{n_u}$. If we suppose that the full state x can be measured, then in the batch NMPC (Nagy et al., 2004) the control input applied to the system in the interval $[t_k, t_f]$ is given by the repeated solution of the finite horizon optimal control problem given by:

$$\min_{\bar{u}(\cdot)} \mathcal{H}(\bar{x}(t), \bar{u}(t)) \tag{20}$$

$$\begin{aligned} s.t.\quad & \dot{\bar{x}}(\tau) = f(\bar{x}(\tau), \bar{u}(\tau)),\ \bar{x}(t_k) = x(t_k) \\ & \bar{u}(\tau) \in \mathcal{U},\ \forall \tau \in [t_k, t_f] \\ & \bar{x}(\tau) \in \mathcal{X},\ \forall \tau \in [t_k, t_f] \\ & \bar{y}(\tau) \in \mathcal{Y},\ \forall \tau \in [t_k, t_f] \end{aligned} \tag{21}$$

where the objective function has the generic form,

$$\mathcal{H}(\bar{x}(t), \bar{u}(t)) = \mathcal{M}(x(t_f)) + \int_{t_k}^{t_F} \mathcal{L}(\bar{x}(\tau), \bar{u}(\tau)) d\tau \tag{22}$$

which consists of the end-point objective ($\mathcal{M}$) and a path term ($\mathcal{L}$), t_k denotes the sampling instance, t_f is the batch time and $t_F \le t_f$ is the prediction horizon for the running term. Although in the case of typical batch NMPC only the end-point objective is considered, based on the nature of the control objective in practical cases often either or both terms may be incorporated in the actual objective function. When $t_F = t_f$ the optimization is performed on a shrinking horizon, whereas if $t_F \le t_f$ initially the problem is solved on a combination of shrinking and moving horizon until $t_k + t_F < t_f$ after which on shrinking horizon. The bar in the optimization problem denotes the predicted variables, i.e. $\bar{x}$ denotes the solution of the system driven by the input $\bar{u}$ with the initial condition $x(t_k)$. Even if in the case of shrinking horizon NMPC in the nominal case the real state x of the system coincides with the predicted state $\bar{x}$, it is necessary to make a distinction between the two due to differences which occurs due to uncertainties in model parameters, inputs and disturbances.

The repeated optimization problem is solved by formulating a discrete form, that can be handled by conventional solvers (Biegler and Rawlings, 1991). The batch time $t \in [0, t_f]$ is divided into N equally spaced time intervals Δt (stages), with discrete time steps $t_k = k\Delta t$, and $k = 0, 1, \ldots, N$. The solution of the optimal control problem is based on the control vector parameterization using a piecewise-constant approximation over equally spaced intervals (Edgar and Himmelblau, 1988). The optimal control problem is solved in the sequential way, the numerical optimizer is the pattern search algorithm (Audet and Dennis, 2002), and the path constraint (maximum liquid level) violation is included in the objective function (Vassiliadis et al., 1994).

The main idea of the shrinking horizon on-line control algorithm is illustrated summarized as follows:

1. with known initial conditions, discretize batch time in N intervals;
2. optimize property at the end of the batch;
3. implement calculated input for the first control interval;
4. initialize optimization with states taken at the end of time interval k;
5. re-optimize property at the end of the batch, having N-1 decision variables in the optimal control problem;
6. implement the first control input;
7. go back to step 4, and repeat until the end of batch.

4. RESULTS AND DISCUSSION

Simulation results are presented using a model which was fitted to a real industrial process with a 6.3 m^3 reactor. The level set point is at a height of 2.1 m. The objective function is to maximize the component B depletion at the end of the batch and the control variable is the temperature. The inequality path constraint is the true reactor level and is incorporated by penalizing the objective function.

The optimal control problem in discrete time step k is formulated as follows:

$$\min_{T(k),\ldots,T(N)} \{n_B(t_f) + C\int_{t_k}^{t_f} \max(0, H - H_{\max})dt\} \tag{23}$$

subject to:

$$T(j) \le T_{\max}, \quad j = k,\ldots,N \tag{24}$$

where n_B is the component B mol number (kmol), C is a large scalar, $H_{\max} = 2.1\,m$ is the maximum level in the reactor and $T_{\max} = 623\,K$ is the maximum temperature. In order to have a comparison basis the catalyst profile in the reactor for the nominal case (Figure 2) and the off-line calculated optimal temperature profile are presented (Figure 3). It can be seen that in the nominal case the open loop control is able to maintain the reactor within the desired safety operating constraints without swelling.

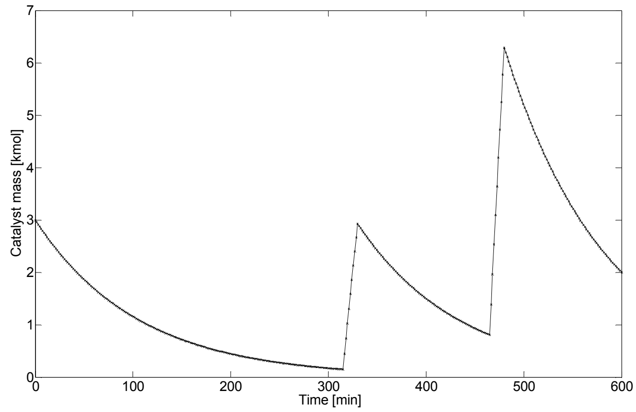

Fig. 2 Catalyst mass in the reactor with feeding shots based on the master recipe (second shot at 310 min, third shot at 460 min).

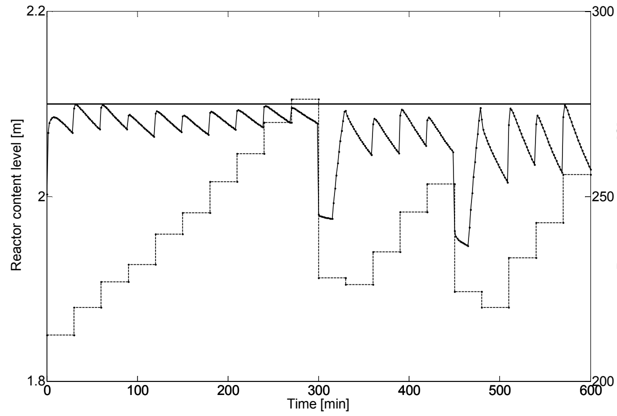

Fig. 3 Off-line calculated optimal temperature profile (dashed line) and corresponding level (continuous line) based on the master recipe catalyst feeding policy (nominal case).

To simulate operating uncertainties a scenario (scenario 1) was considered, in which the catalyst is fed sooner and in smaller quantity than required by the nominal recipe. The changed catalyst feeding policy is shown in Figure 4.

The Figure 5 represents the control performance when the optimal temperature profile determined off-line is applied in the case of scenario 1 (disturbance in operating recipe). It can be seen that deviations from the nominal operating recipe can yield significant violation of the maximum level leading to productivity lost and even safety hazard. The reactor level increases over the maximum level between 200-300 min and 400-500 min, respectively. Additionally, suboptimal process operation is carried out between 300-400 min and 450-600 min (the temperature could be higher which would lead to faster reaction rates).

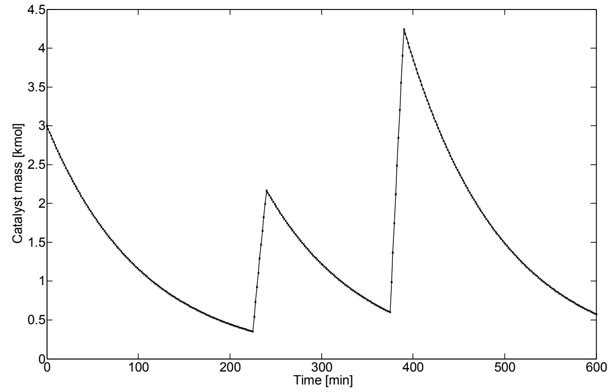

Fig. 4 Changed catalyst feeding policy; the catalyst is fed sooner (second shot at 220 min, third shot at 380 min) and in smaller mass (scenario 1).

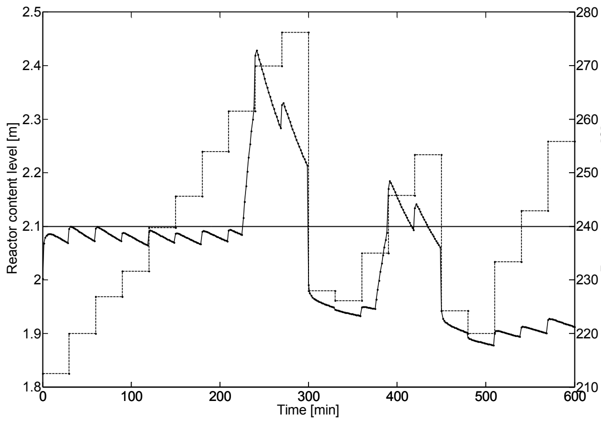

Fig. 5 Simulation using the off-line calculated optimal temperature profile with a new catalyst dosing strategy (scenario 1).

The results obtained with the implemented on-line model based control strategy are presented in Figure 6. The on-line optimization based control strategy is able to adapt the temperature profile to avoid the violation of the level constraint during most of the batch. When the disturbance occurs within sampling times violation of the maximum level constraint can still be observed due to the lack of feedback between sampling instances.

A second scenario (scenario 2), when the catalyst is fed with delay and in larger quantities, was also considered. The feeding policy in this case is shown in Figure 7. The results obtained with the on-line optimization based control strategy are shown in Figure 8. The batch NMPC was able to adapt the control input to the new feeding scenario minimizing the effect of disturbances from the recipe.

Based on the results presented above we can conclude that the on-line model based control was able to keep the reactor level at the set-point without causing excessive swelling or sub-optimal operation for most of the batch even in the case of significant deviations from the master recipe.

However, the NMPC does not always provide sufficiently good level control between two sampling times. This is due to the fact that the controller actions are fixed on a control interval, thus the new disturbances are taken into account only at the next sampling time. After the next sampling time the controller is able to reject the disturbance.

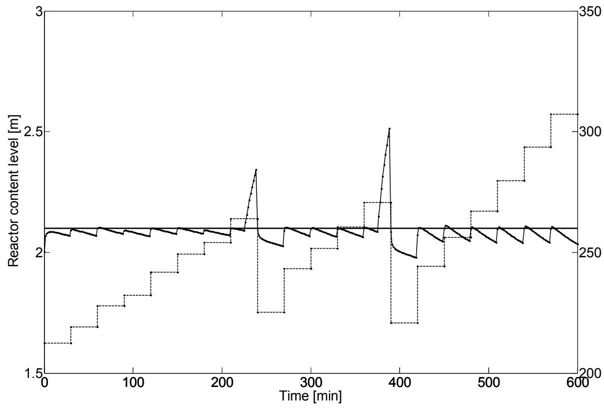

Fig. 6 Optimal temperature profile and resulting reactor level in the case of batch NMPC for the catalyst feeding presented in scenario 1.

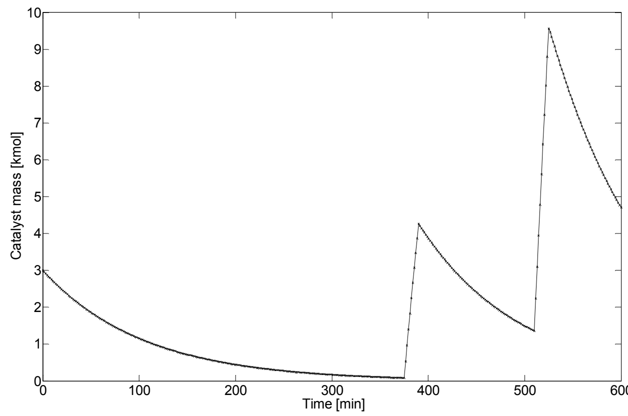

Fig. 7 Changed catalyst feeding policy; the catalyst is fed later (second shot at 380 min, third shot at 510 min) and in larger mass (scenario 2).

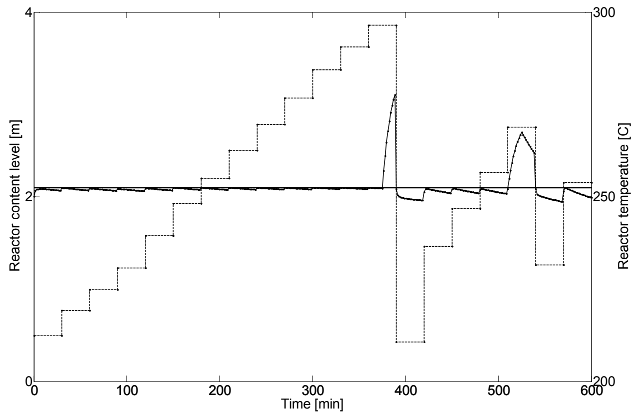

Fig. 8 Optimal temperature profile and resulting reactor level in the case of batch NMPC for the catalyst feeding presented in scenario 2.

The problems generated by the lack of feedback between optimization sampling times can be minimized by decreasing the sampling times. However, in the case of batch NMPC with end-point objective, the entire batch time has to be considered which can lead to a large optimization problem. Since the level measurement is in practice instantaneous in this application another solution would be to "sense" the disturbance, which would trigger the recalculation of the control action immediately when the violation of the constraint is detected. Alternatively, a closed-loop NMPC can be implemented. In this case the optimization repeatedly finds a feedback law rather than an open-loop profile. The simplest control law is a linear output feedback level controller:

$$T(t) = K(k)(H_{set} - H(t)) \tag{25}$$

where, *K(k)* is the controller gain which is fixed on a discretization interval, and is the result of the closed-loop NMPC optimization problem. This approach could not improve the level control and induced level oscillations; this is due to the time varying feature of the catalyst concentration during the feeding period, and to the non-linear temperature influence on the reactor level. Finally, a practical approach was also considered: prior any catalysts feeding in the reactor, the temperature must be decreased to a certain safe set point (by this the calculated NMPC action is discarded); this value needs to be determined so that is able to accommodate any disturbance of the reaction rate. Although this approach is sub-optimal, it is a safe procedure to cope with the reaction rate uncertainty, as presented in Figure 9. In this case the role of the NMPC is to start the reaction in a safe and optimal way after each catalyst dosing.

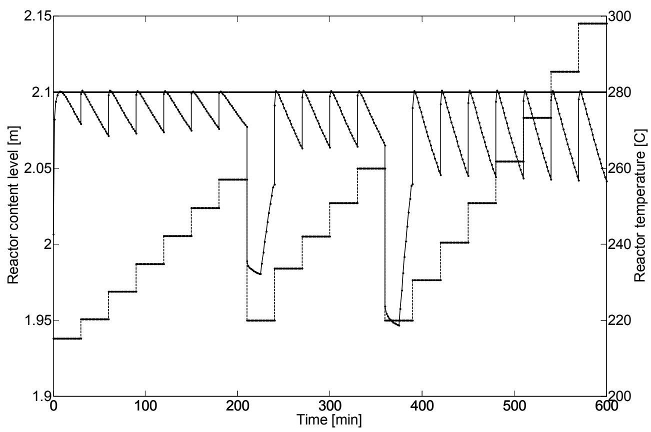

Fig. 9 The NMPC action override strategy and the reactor level.

5. CONCLUSIONS

This work presents the non-linear model based level control of a batch reactor. The on-line strategy is required to accommodate the reaction rate disturbances which arise due to catalyst dosing uncertainties (catalyst mass and feeding time). It is concluded that the implemented shrinking horizon on-line optimization strategy is able to calculate the optimal temperature profile without causing swelling or sub-optimal operation. Additionally, the presented investigation outlines the potential control difficulties of the NMPC strategies within a sampling interval.

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