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Model based control of a liquid swelling constrained batch reactor subject to recipe uncertainties

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ABSTRACT

This work presents the application of nonlinear model predictive control (NMPC) to a simulated industrial batch reactor subject to safety constraint due to reactor level swelling, which can occur with relatively fast dynamics. Uncertainties in the implementation of recipes in batch process operation are of significant industrial relevance. The paper describes a novel control-relevant formulation of the excessive liquid rise problem for a two-phase batch reactor subject to recipe uncertainties. The control simulations are carried out using a dedicated NMPC and optimization software toolbox *OptCon* which implements efficient numerical algorithms. The open-loop optimal control problem is computed using the multiple-shooting technique and the arising nonlinear programming problem is solved using a sequential quadratic programming (SQP) algorithm tailored for large-scale problems, based on the freeware optimization environment HQP. The fast response of the NMPC controller is guaranteed by the initial value embedding and real-time iteration technologies. It is concluded that the *OptCon* implementation allows small sampling times and the controller is able to maintain safe and optimal operation conditions, with good control performance despite significant uncertainties in the implementation of the batch recipe.

1. Introduction

Reactor or evaporator content swelling phenomena can lead to significant productivity losses if this phenomenon is not considered during process operation and is regarded as a reactor productivity and safety problem. Reactor content swelling occurs when the vessel content level rises due to a gas or vapor stream that passes through the liquid (Fig. 1). Vapor flow occurs in a reactor when the reaction produces a gas phase product or during 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). The off-line optimal temperature control of batch reactors with regard to swelling was subject of investigation by Simon et al. [1]. Similarly to the batch reactors, reboiler liquid swelling may also occur during the operation of low-pressure batch distillation processes [2].

Since the advent of dynamic matrix control (DMC), model predictive control (MPC) has been the most popular advanced control strategy in the chemical industries [3]. Linear MPC has been heralded as a major advance in industrial process control [4]. 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 [5]. Nonlinear model predictive control (NMPC) reformulates the MPC problem based on nonlinear process models, providing the advantage to cope inherently with process nonlinearities [6,7] characteristic to batch systems. Recent developments in the field of real-time optimization use the feedback information to adapt the constraints of the optimization problem instead of updating the model parameters [8]. On-line optimization and integration of extended Kalman filter based estimation was shown to be an effective way to increase productivity of exothermic batch reactors [9]. Recent predictive control formulations that explicitly account for process nonlinearities and do not require the traditional assumption of initial feasibility of the optimization problem are presented by Refs. [10,11]. Zavala and Biegler proposed the advanced-step NMPC controller to reduce the on-line computational effort via the reformulation of the NMPC problem [12]. New challenges related to the optimal transition from batch to continuous processing of bio-reactors, are handled using a nonlinear model predictive controller to ensure the constraints satisfaction and performance targets [13]. Although not considered in this paper robust formulations that incorporate parameter

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Nomenclature

Latin symbols

c_{Hydro}^{Model}	vector of hydrodynamic model specific constants and parameters
c_{R}^{Model}	vector of reactor model specific constants and parameters
dn	vector of accumulation or consumption rates of all components (kmol/s)
E_{Cat}	catalyst deactivation reaction activation energy (kJ/kmol)
$E_{A,i}$	activation energies (kJ/kmol)
f	hydrodynamic model constant
F_{Cat}	catalyst dosing rate (kmol/s)
G	set of dynamic equations and set of equality constraints
H	swelled vessel height (m)
H_0	height of the resting liquid (m)
H_{max}	maximum reactor level (m)
$Hydro$	hydrodynamic model
j_g	vapor superficial velocity (m/s)
K	hydrodynamic model constant
K_c	dynamic controller gain
k	discretization interval
k_{Cat}	rate constant at reference temperature (m^3/(kmol s))
k_{ref}^{i}	rate constants at reference temperature (m^6/(kmol^2 s))
M	objective function
$n_A, n_B, n_C, n_D, n_E, n_F, n_P, n_W$	mole number of component A, B, C, D, E, F, P, W (kmol)
N	number of intervals
R	gas constant (kJ/(kmol K))
r_{Cat}	catalyst deactivation rate (kmol/(m^3 s))
$\Re^n$	set of inputs, states, outputs
r_R^i	ith reaction rate to the right-hand side (kmol/(m^3 s))
T	reactor temperature (°C)
T_{ref}	reference temperature (°C)
t_f	final time (s)
U_∞	characteristic bubble rise velocity (m/s)
u	input
V	reactor mass volume (m^3)
V_g	average local slip velocity (m/s)
x	states
$\bar{x}$	predicted state
y	output

Greek letters

$\bar{\alpha}$	pool void fraction
ρ_L	liquid density (kg/m^3)
ρ_V	vapor density (kg/m^3)
Ψ	path term
σ	surface tension (N/m)

Superscripts

1	Reaction 1
2	Reaction 2
3	Reaction 3
4	Reaction 4

Subscripts

Cat	catalyst
i	ith reaction step
ref	reference

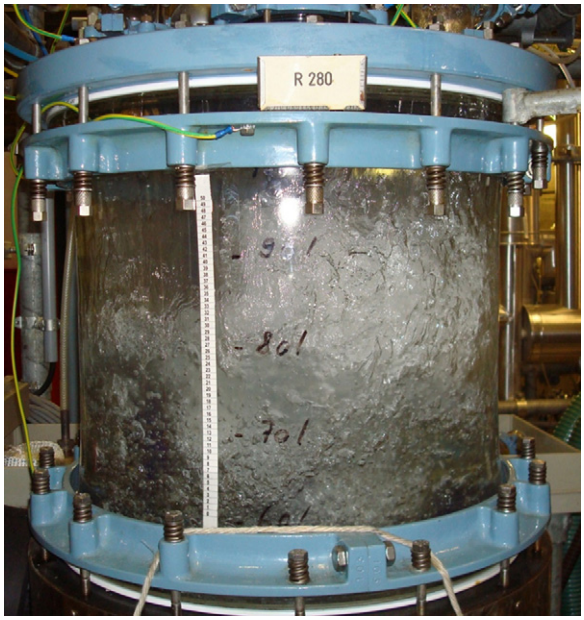

Fig. 1. Swelled liquid in a 100 L pilot plant vessel.

uncertainties in the control problem formulation are also available [14,15], and their application for the case of recipe uncertainties represents an interesting future research problem due to its relevance to the industrial batch processes operations.

Typically, the dynamics of the systems encountered during the processing of chemicals such as reactions, separations are relatively slow, with time constants of the order of minutes. The novelty of the paper is that it illustrates the benefits of application of an efficient on-line optimizing nonlinear model based control approach to a chemical process with fast dynamics, a reactive-hydrodynamic system. The model based control approach is justified by the time varying nature of the batch process, by the nonlinearities due to the chemical system and the necessity of constraint handling. The on-line strategy is required to accommodate the reaction rate disturbances which arise due to catalyst dosing uncertainties (catalyst mass and feed time). The optimization problem is implemented in a user-friendly software package, *OptCon* [16,17].

2. Process operation and models

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 catalyst dosing takes place at the beginning of the operation, later 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. Fig. 2 shows the experimental reaction rate measurements (normalized data) from the real industrial plant, in the case of repeated application of the same operating recipe with two consecutive catalyst dosing. The significant bath-to-batch variation may lead to safety problems and sub-optimal operation.

The process recipe is optimized off-line by calculating the catalyst dosing time and mass, and the optimal pressure profile which ensures that the liquid level is at the setpoint. However, the off-line calculated optimal pressure profile does not ensure safe operation in the case of disturbances in the catalyst feeding policy. Instead, an on-line strategy is needed to adjust the pressure profile during the

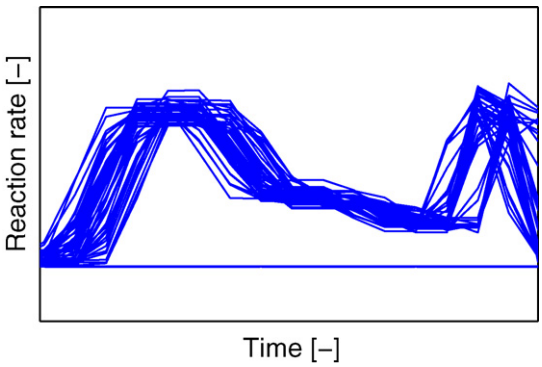

Fig. 2. Change of the reaction rate in time for an existing batch process.

operation considering the unknown disturbances. The control strategy used here is based on the nonlinear model predictive control (NMPC) framework for batch processes.

2.1. Batch reactor modeling

Four equilibrium reactions in series take place in the liquid phase and a catalyst is used in dissolved form. The reaction scheme is as follows:

$$A + B \xrightarrow{k^1_{ref}} C + D \quad (1)$$

$$B + C \xrightarrow{k^2_{ref}} E + D \quad (2)$$

$$B + E \xrightarrow{k^3_{ref}} F + D \quad (3)$$

$$B + F \xrightarrow{k^4_{ref}} P + D \quad (4)$$

$$B + \text{Catalyst} \xrightarrow{k_{Cat}} W \quad (5)$$

Raw materials are component A and B, while C, E, F are intermediates, P is the desired product and W is the decomposed catalyst. The goal of the process operation is to remove the co-product D from the liquid phase as fast as possible to shift the equilibrium reactions to the product side. 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 and implicitly on the formation rate of gas co-product D.

By operating at low-pressure conditions, the amount of D in liquid phase is minimized, thus the reverse reactions are not significant. Although the reaction system is characterized by chemical equilibrium, the chemical model is based only on forward reactions which ensure a safety back-off in the model. The true reaction rates will never be faster than the forward reactions.In order to model the forward reactions the Arrhenius formulation is implemented, using a reference reaction constant determined at a reference temperature [18]:

$$r^i_R = k^i_{ref} \exp\left\{-\frac{E_{A,i}}{R}\left(\frac{1}{T_r} - \frac{1}{T_{ref}}\right)\right\} \frac{n_{Cat} n_B n_X}{V^3} \quad (6)$$

$$r_{Cat} = k_{Cat} \exp\left\{-\frac{E_{Cat}}{R}\left(\frac{1}{T_r} - \frac{1}{T_{ref}}\right)\right\} \frac{n_{Cat} n_B}{V^2} \quad (7)$$

where i is the ith reaction step, r^i_R is the ith reaction rate to the right-hand side (kmol/(m^3 s)), r_{Cat} is the catalyst deactivation rate, k^i_{ref} are the corresponding rate constants at reference temperature (m^6/(kmol^2 s)), k_{Cat} is the catalyst deactivation rate constant at reference temperature (m^3/(kmol s)), $E_{A,i}$ the activation energies (kJ/kmol), E_{Cat} the catalyst deactivation reaction activation energy (kJ/kmol), T_r and T_{ref} are the current and reference temperature (K), R is the gas constant (kJ/(kmol K)), n_B is the mole number of component B (kmol), n_{Cat} is the catalyst mole number (kmol), n_X represents n_A, 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 as a 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:

$$\frac{dn_A}{dt} = -r^1_R V \quad (8)$$

$$\frac{dn_B}{dt} = (-r^1_R - r^2_R - r^3_R - r^4_R - r_{Cat})V \quad (9)$$

$$\frac{dn_C}{dt} = (r^1_R - r^2_R)V \quad (10)$$

$$\frac{dn_D}{dt} = (r^1_R + r^2_R + r^3_R + r^4_R)V \quad (11)$$

$$\frac{dn_E}{dt} = (r^2_R - r^3_R)V \quad (12)$$

$$\frac{dn_F}{dt} = (r^3_R - r^4_R)V \quad (13)$$

$$\frac{dn_P}{dt} = r^4_R V \quad (14)$$

$$\frac{dn_{Cat}}{dt} = -r_{Cat}V + F_{Cat} \quad (15)$$

where F_{Cat} is the catalyst dosing rate (kmol/s). In a previous work the mass of component D in liquid phase during boiling under vacuum was inferred using a hybrid black-box model [19].

2.2. Void fraction modeling

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 the following equation:

$$H = \frac{H_0}{1 - \bar{\alpha}} \quad (16)$$

Wilson et al. [20] determined the void fraction $\bar{\alpha}$ by bubbling steam through water in a pressurized vessel in the 20–40 bar pressure range. Their proposed empirical correlation is presented below:

$$\bar{\alpha} = K\left(\frac{\rho_V}{\rho_L - \rho_V}\right)^{0.17}\left[\sqrt{\frac{\sigma}{g(\rho_L - \rho_V)}}/D_{reb}\right]^{0.1} \left[j_V \Big/ \left(g\sqrt{\frac{\sigma}{g(\rho_L - \rho_V)}}\right)^{0.5}\right]^f \quad (17)$$

with

$$K = 0.68, \quad f = 0.62 \qquad \text{for} \; j_V \Big/ \left(g\sqrt{\frac{\sigma}{g(\rho_L - \rho_V)}}\right)^{0.5} < 2 \quad (18)$$

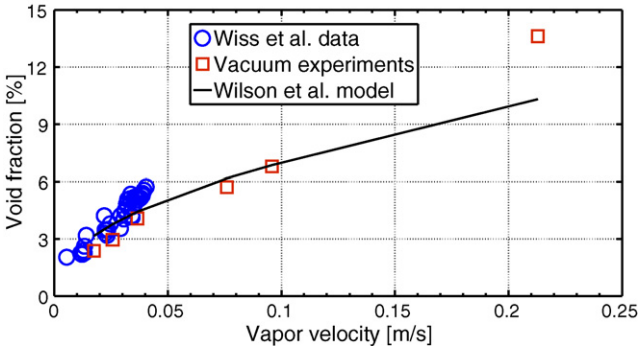

Fig. 3. Void fraction prediction using the Wilson model [25].

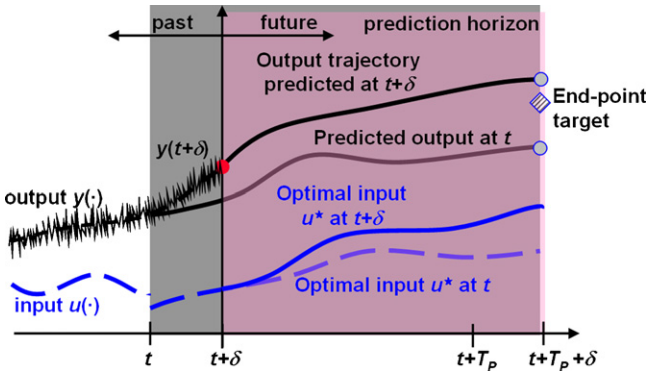

Fig. 4. The concept of shrinking horizon NMPC strategy.

$$K = 0.88, \quad f = 0.40 \qquad \text{for} \, j_V \Big/ \left(g \sqrt{\frac{\sigma}{g(\rho_L - \rho_V)}} \right)^{0.5} \geq 2 \tag{19}$$

where ρ_L and ρ_V (kg/m^3) are the liquid and vapor densities, σ (N/m) is the surface tension, g (m/s^2) is the gravitational acceleration, D_{reb} (m) is the reboiler vessel diameter and j_V (m/s) is the superficial vapor velocity, K and f are model specific constants. The comparison of the void fraction predictions as a function of the gas flow rate using the four hydrodynamic models is discussed in Simon et al. [2]. It is concluded that, at 1 bar pressure, the Wilson and Churn turbulent [21] and Sterman models [22] show similar behavior, and the Kataoka–Ishii model [23] predicts larger void fractions. The four hydrodynamic models were compared at 0.25 bar pressure as well; the comparison results show that the Wilson and Churn turbulent model predictions are similar, while the Sterman and Kataoka–Ishii models predict larger void fractions. It is interesting to note that the Wilson model was successfully extrapolated by Wiss et al. [24] (without refitting the model parameters) from about 20–40 bar pressure to 1 bar. To the authors' knowledge void fraction correlations identified under vacuum conditions are not available in the literature, therefore experiments within 0.1 and 0.8 bar were carried out [25]. It was found that at 0.1 bar, the Wilson model predicts correctly the void fraction values up to 10–15%, as shown in Fig. 3. In conclusion, the Wilson model is a good choice for pool boiling modeling under vacuum conditions, thus it is used in the model applied in the current calculations. For the in situ, laboratory scale monitoring of hydrodynamic conditions endoscopy assisted by digital image processing can be a useful approach [26,27].

3. On-line optimizing control for swelling constrained batch reactor

The on-line optimizing control for a model represented by a generic ordinary-differential equation (ODE) system can be expressed as follows:

$$\dot{x}(t) = f(x(t), u(t)) \tag{20}$$

$$y(t) = g(x(t), u(t)) \tag{21}$$

subject to the input, state and output constraints

$$u(t) \in U, \qquad x(t) \in X, \qquad y(t) \in Y \tag{22}$$

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 X and Y are closed subsets of $\Re^{n_x}$ and $\Re^{n_y}$, respectively and the set U is a compact subset of $\Re^{n_u}$. If we suppose that the full state x can be measured, then in the batch NMPC [16,17] 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:

$$\min_{\bar{u}(\cdot)} \left\{ M(x(t_f)) + \int_{t_k}^{t_F} \Psi(\bar{x}(t), \bar{u}(t)) \, dt \right\} \tag{23}$$

$$\begin{aligned} \text{s.t.} \quad & \dot{\bar{x}}(t) = f(\bar{x}(t), \bar{u}(t), \bar{x}(t_k) = x(t_k)) \\ & \bar{u}(t) \in U, \quad \forall t \in [t_k, t_f] \\ & \bar{x}(t) \in X, \quad \forall t \in [t_k, t_f] \\ & \bar{y}(t) \in Y, \quad \forall t \in [t_k, t_f] \end{aligned} \tag{24}$$

where the objective function has the generic form, which consists of the end-point objective (M) and a path term (Ψ), t_k denotes the sampling instance, t_f is the batch time and $t_F \leq t_f$ is the prediction horizon for the running term, and τ is the model time. A schematic representation of the principle of batch NMPC is given in Fig. 4. 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 one 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 $t_F \leq t_f$ 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 occur 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 [28]. 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 main idea of the shrinking horizon on-line control algorithm (batch NMPC) is shown in Fig. 4 and is 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.

The solution of the optimization problem is implemented in a dedicated NMPC tool, *OptCon* [16]. In particular, the NMPC is based on first-principles or grey box models, and the problem setup can be

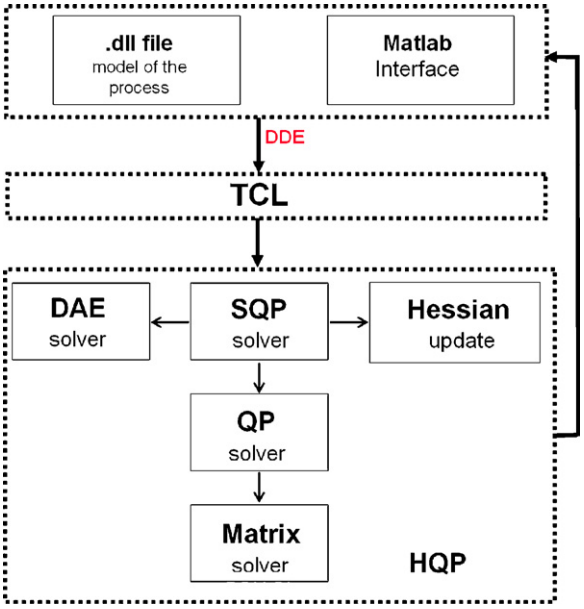

Fig. 5. The *OptCon* structure.

done in Matlab. The NMPC approach is based on a large-scale NLP solver (HQP) [17,29] which offers an efficient optimization environment, based on multiple-shooting algorithm [30,31], that divides the optimization horizon into a number of subintervals (stages) with local control parameterizations. The differential equations on these intervals are integrated independently during each optimization iteration. The continuity/consistency of the state trajectory at the end of the optimization is enforced by adding consistency constraints to the nonlinear programming problem. The basic components of the software package and the working mechanism are shown in Fig. 5. The software consists of a collection of ODE/DAE solvers, SQP solvers, QP solvers, matrix solver for the solution of the Karush–Kuhn–Tucker (KKT) condition and various methods for Hessian update, all compiled together in a dynamically link library (dll). The model has to be implemented as a standard Matlab mex function using C language and compiled also as a dll. Communication between the optimization functions and model function is performed via the open source TCL shell in a client/server structure. Communication functions and high level configuration and NMPC functions are developed in Matlab so that the structure of the package is completely transparent to the user. The user only interacts with the functions in Matlab and sets up the optimization, parameter and/or state estimation, and NMPC problems using the Matlab interface. The NMPC and estimation functions in *OptCon* are designed using a special real-time scheme and the software also offers the possibility to be connected to real distributed control systems (DCS) through OPC communication.

Hence OptCon provides an efficient environment for rapid prototyping of NMPC strategies even in an industrial environment and has been successfully used in a variety of practical applications [17].

4. Results and discussion

4.1. Open-loop optimal control of the swelling constrained batch reactor

The most widely used optimization method to improve the batch processes is the formulation and solution of an optimal control problem [32]. The open-loop optimization problem corresponds to the first optimization step in the batch NMPC algorithm described in the previous section. In this approach the objective is to improve an end-point criteria by calculating a time variant input variable profile (temperature, pressure, feed rate).

Since the reactions are chemical equilibrium limited it is important that the pressure in the reactor is the lowest possible. However, minimum reactor pressure yields maximum gas volume and eventually maximum liquid level, thus this limitation has to be taken into account during the calculation of the pressure profile. Although it is plausible to control the cause of the vapor formation (reaction kinetics) using the temperature, in practice this is not possible due to the slow dynamics of temperature change in large-scale reactors. Instead, from practical point of view, it is more feasible to control the true level by means of the pressure. For this case study the temperature ramp is set to 1 °C/min. The temperature is an additional state in the model and it is not considered as a disturbance in the system, however the pressure re-optimization takes into account possible changes, as it affects the reaction rate, the vapor velocity and the true level.

The optimization of the batch reactor with regard to swelling can be regarded as a problem to determine the pressure profile which will not cause the level to rise over a maximum value. The objective function is to maximize the component B depletion or to minimize the content of component B at final time, the control variable is the pressure, and the final simulation time is fixed to 40 min. The inequality path constraint is the formation rate of co-product D converted in true reactor content level. The optimal control problem for this process is formulated as follows:

$$M = \min_{P(t)} \int_0^{t_f} P(t)\ dt \tag{25}$$

Subject to:

$$g(Rdae(\dot{x}, x, T, \nu_R, c_R^{Model}), Hydro(\dot{x}, T, P, \nu_R, c_{Hydro}^{Model}), t_f, t) = 0 \tag{26}$$

$$H_{max} - H_r(t) \geq 0 \tag{27}$$

$$P_{max} - P(t) \geq 0 \tag{28}$$

$$P(t) - P_{min} \geq 0 \tag{29}$$

where t_f is the final time (end of the optimization) at which it is considered that swelling cannot occur anymore (not yet the end of the reaction), P is the pressure proposed by the optimizer, *Rdae* is the kinetic model, ν_R is the vector of reaction mass specific constants, c_R^{Model} is the vector of reaction model specific parameters, *Hydro* is the hydrodynamic model, c_{Hydro}^{Model} is the vector of hydrodynamic model specific constants and parameters, H_{max} (2.4 m) and H_r (t) are the maximum level and calculated reactor content level, respectively, and P_{max} (1 bar) and P_{min} (0.075 bar) are the maximum and the minimum pressures, respectively. The objective function is expressed as the integral of the pressure profile over the batch time. This formulation guaranties that the maximum level is not exceeded while the pressure is kept at the minimum possible level, which indirectly maximizes productivity. Fig. 6a shows the open-loop optimal pressure profile and Fig. 6b the calculated reactor level. The pressure increases due to the catalyst feeding procedure which takes place during short periods at time steps 0, 15, 25, 35 min during which the reaction rate increases. However, during the operation of the batch reactor there is an uncertainty regarding the catalyst mass and dosing time which causes significant level increase and sub-optimal operation. Furthermore, Fig. 6b shows the true reactor level in case when the catalyst is dosed 3 min earlier compared to the recipe and also considering that 20% more mass is added. The sampling time is 20 s. In the industrial practice the pressure increase for processes operated under vacuum is implemented by opening a valve placed before the vacuum pump.

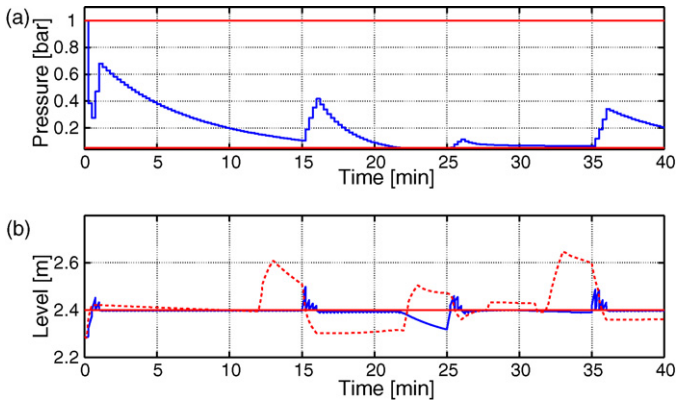

Fig. 6. Open-loop calculated pressure profile (a) and the corresponding reactor level (b), straight lines; dashed line shows the reactor level according to the disturbed conditions. Catalyst dosing at 15 min, 25 min and 35 min.

4.2. On-line re-optimizing control of the swelling constrained batch reactor

In order to cope with the disturbance of the chemical system a shrinking horizon, re-optimizing model based control strategy is implemented. The optimal control problem defined by Eqs. (25)–(29) is solved repeatedly considering a state feedback formulation. This assumption is used since in practice the concentrations (states) are measurable with spectroscopy based techniques such as infrared (IR) and ultra-violet visible (UV/vis) spectroscopy [33]. The measured spectra are previously calibrated to known concentration samples using partial-least squares (PLS) models.

Besides the states presented in Eqs. (8)–(15), further states for the temperature, total dosed catalyst mass, mass of component B consumed in the main reaction and a state for the pressure integral have been included. The size of the first NLP is 1560 variables which is calculated as follows: the batch time is 2400 s and with a 20 s sampling time leads to 120 discretization intervals. Since in the multiple-shooting scheme the control variables and the states are discretized the number of unknowns in the NLP is given by $120 \times 12 + 120$. The first open-loop optimization is completed in about 10 s and 13 QP iterations (relative integration error: 1e−3; absolute integration error: 1e−6). After each re-optimization the NLP size decreases with 13 variables. Subsequent optimizations, when disturbances are not present, are carried out in about 1–2 s and 2 QP iterations since the NLP is initiated from the previous optimization results. The calculations were carried out using an Intel Centrino vPro processor at 2.5 MHz frequency with 4GB installed random access memory (RAM) on a Windows XP operation system.

The level control results for the case when the catalyst is fed 3 min earlier and 20% more mass than specified by the recipe is presented in Fig. 7. Due to the small sampling time the controller is able to accommodate the change of vapor rate and it maintains the level at the maximum level. In this case the information contained in the original recipe is not used by the model during the open-loop optimization, since the catalyst dosing is expected later.

Further simulations deal with the case when the catalyst is fed delayed and with 20% more mass as set in the recipe. Fig. 8 presents the case when the catalyst feed is delayed 3 min. Similarly to the previous case the level control is good despite the disturbance in the recipe.

In order to analyze the effect of the recipe information on the process control behavior a scenario was simulated in which the catalyst feeding time is delayed 30 s (the catalyst feeding takes 1 min). This way it is expected that the controller has information about the dosing time in the open-loop optimization. This expectation is confirmed in Fig. 9b, where it is observed that the level is lower within the first sampling time.

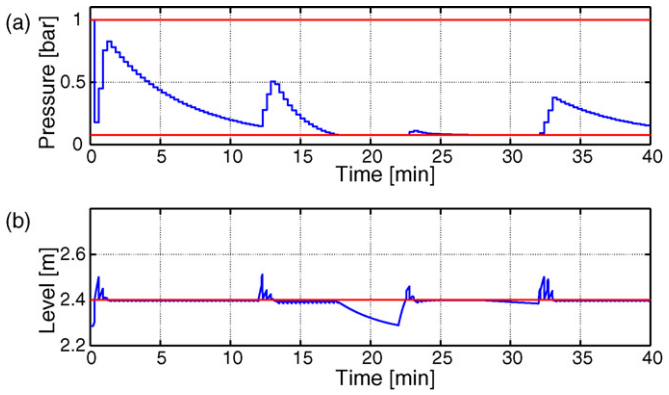

Fig. 7. Pressure profile (a) and the corresponding reactor level for an early addition disturbance case. Catalyst dosing at 12 min, 22 min and 32 min.

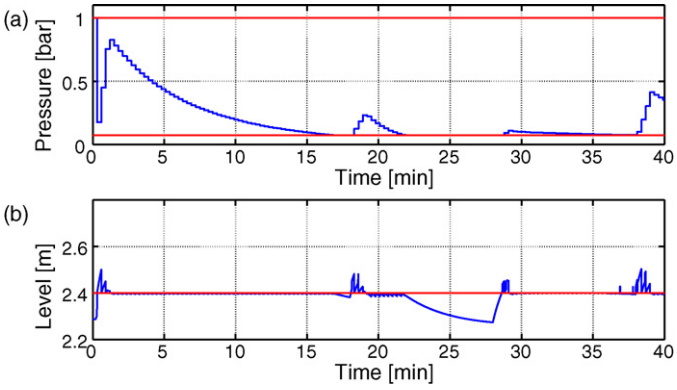

Fig. 8. Pressure profile (a) and the corresponding reactor level for a late addition (with 3 min) disturbance case. Catalyst dosing at 18 min, 28 min and 38 min.

In order to verify the influence of the model–plant mismatch, a slower, thus conservative model was used. In the kinetic model the activation energies were increased by 30% and the prediction of the hydrodynamic model was decreased by 30%. This way the true level height is under predicted. The simulation results considering early catalyst feeding (3 min sooner) and the model discussed above are presented in Fig. 10. An offset compared to the maximum level is observed, which can be decreased by running the optimization problems with the level constrained at 2.3 m. Using a model which under predicts the level the optimizer will try to lower the pressure to a higher extent compared to the prediction which is based on an accurate model. For low pressures the effect of plant–model mis-

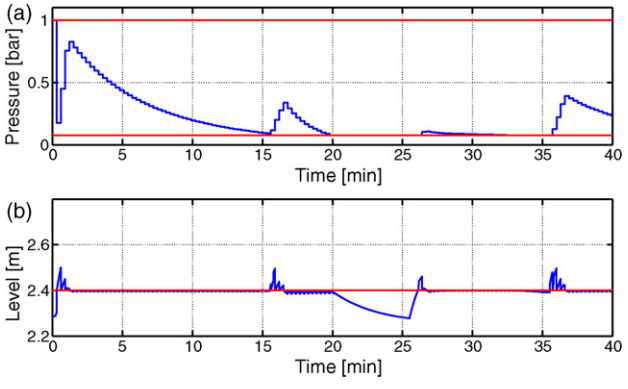

Fig. 9. Pressure profile (a) and the corresponding reactor level for a late addition (with 30 s) disturbance case (b). Catalyst dosing at 15.5 min, 25.5 min and 35.5 min.

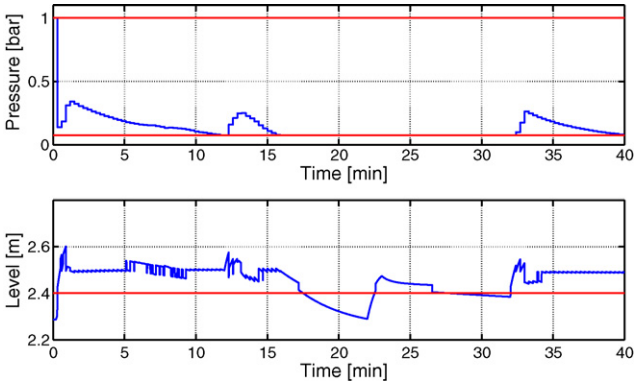

Fig. 10. Pressure profile (a) and the corresponding reactor level (b) for an early addition (with 3 min) disturbance case, using a model with significant model–plant mismatch. Catalyst dosing at 12 min, 22 min and 32 min.

match is controlled by the lower bound on the pressure which is the control variable. As shown in the results presented above using small sampling time the control performance is good.

There are cases when the NMPC strategy may not allow the implementation of small sampling time control actions. In these cases the open-loop formulation of the NMPC control problem, according to which the NMPC control actions are applied in an open-loop way between the NMPC sampling instances, may not provide acceptable results. During the open-loop control period a disturbance may lead to the rapid rise of the reactor level and hence to the violation of safety constraint. In these cases a closed-loop NMPC can be implemented. According to this strategy the optimization repeatedly finds a feedback law rather than an open-loop profile. The simplest control law is a linear output feedback level controller,

$$P(t) = K_c(k)(H_{set} - H(t)) \tag{30}$$

where $K_c(k)$ is the dynamic controller gain which is fixed on a discretization interval and is the result of the closed-loop NMPC optimization problem [34]. This control strategy is based on reliable level sensors which provide reliable level measurements despite boiling conditions. As an alternative to existing level measurement solutions, external, digital imaging based level monitoring can be considered [35].

4.3. Process safety by design and feedback control

Often, process disturbances are handled during the design phase by increasing the size of the equipment. The same strategy is used to account for the uncertainties of correlations and model parameters which influence equipment sizing. Another safe alternative is to use high filling degree and set the base case recipe so that disturbances do not cause safety problems [36]. Although inherently safe, these practices lead to solutions which decrease the process performance, usually the productivity, as the material throughput is decreased. The level disturbance can also be handled by decreasing the filling level in the reactor. More exactly, for a 6.3 m^3 reactor which has a nominal height of 2 m, decreasing the filling height by 0.5 m, the liquid volume is decreased by 25%. Advanced control solutions can help to provide safe operation and to improve productivity, in this case by filling more liquid. Nevertheless, the implementation of advanced control loops in industrial environments requires not only performant process models and solvers, but also the integration with existing actuators, and last but not least skilled man power to ensure deployment and maintenance. Thus, the costs related to the implementation of advanced control solutions need to be balanced against the productivity benefits.

Related to the modeling simplifications, it is concluded that, assuming fixed batch time, the yield of the reaction might change due to the different pressure profiles which affect the liquid–vapor equilibrium (VLE), the component D hold-up and the reverse reaction rates. As the model does not contain the pressure influence on the liquid hold-up of component D, it is not feasible to quantify the effect of pressure profile change, since VLE calculations are not performed. Uncertainties of the chemical equilibrium constants and the assumption that in large-scale industrial reactors the entire liquid mass is in equilibrium with the gas phase pose further modeling difficulties. In such cases, to model the phase transition, it is customary to postulate rate-based models which do not assume equilibrium.

5. Conclusions

The paper presents an on-line optimizing batch process control strategy with respect to excessive liquid rise. The on-line strategy is required to accommodate the reaction rate disturbances which arise due to catalyst dosing uncertainties (variations in catalyst mass and feeding time). The control simulations are carried out using a dedicated NMPC and optimization software toolbox *OptCon* which implements state of the art technologies. The open-loop optimal control problem is computed using the multiple-shooting technique and the arising nonlinear programming problem is solved using a sequential quadratic programming (SQP) algorithm tailored for large-scale problems, based on the freeware optimization environment HQP. The fast response of the NMPC controller is guaranteed by the initial value embedding and real-time iteration technologies. This efficient NMPC scheme allows the implementation of control actions with small sampling time, which is an important aspect in this application, which may exhibit very rapid rise in level due to swelling. The simulation results obtained using the model fitted to industrial experimental data indicate that the on-line model based control is able to keep the reactor level within safety operation constraints, without causing excessive liquid swelling or sub-optimal operation even in the case of significant deviations from the master recipe. Further process optimization strategies may include on-line recipe adjustment scenarios, in this case, by re-optimizing the catalyst dosing time and mass.

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