# Real-Time Implementation of Nonlinear Model Predictive Control of Batch Processes in an Industrial Framework

Zoltan K. Nagy[1], Bernd Mahn[2], Rüdiger Franke[3], and Frank Allgöwer[4]

[1] Loughborough University, Chemical Engineering Department, Loughborough, LE11 3TU, United Kingdom
Z.K.Nagy@lboro.ac.uk
[2] BASF Aktiengesellschaft, Ludwigshafen, Germany
[3] ABB Corporate Research, Ladenburg, Germany
[4] University of Stuttgart, Stuttgart, Germany

**Summary.** The application of nonlinear model predictive control (NMPC) for the temperature control of an industrial batch polymerization reactor is illustrated. A real-time formulation of the NMPC that takes computational delay into account and uses an efficient multiple shooting algorithm for on-line optimization problem is described. The control relevant model used in the NMPC is derived from the complex first-principles model and is fitted to the experimental data using maximum likelihood estimation. A parameter adaptive extended Kalman filter (PAEKF) is used for state estimation and on-line model adaptation. The performance of the NMPC implementation is assessed via simulation and experimental studies.

## 1 Introduction

Trends in the process industries toward high value added products have increased the interest in the optimal operation of batch processes, used predominantly for high-tech products. Batch processes are common in the pharmaceutical, microelectronics, food, and fine chemical industries. It is widely recognized at industrial level that advanced control techniques have the potential to improve process performance [QB03]. Since the advent of dynamic matrix control (DMC), model predictive control (MPC) has been the most popular advanced control strategy in chemical industries [ML97]. Linear MPC has been heralded as a major advance in industrial control. 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. Nonlinear model predictive control (NMPC) has been considered as one of the most promising advanced control approaches for batch processes. NMPC reformulates the MPC problem based on nonlinear process models. Different nonlinear models can be used for prediction, from empirical black-box models (e.g. artificial neural networks, Volterra series, etc.) to detailed, first-principles based representations of the system, leading to a wide variety of different NMPC approaches [Hen98], [FA02]. The advantages of using complex nonlinear models in the NMPC are

R. Findeisen et al. (Eds.): Assessment and Future Directions, LNCIS 358, pp. 465–472, 2007.
springerlink.com 

straightforward. First-principles models are transparent to engineers, give the most insight about the process, and are globally valid, and therefore well suited for optimization that can require extrapolation beyond the range of data used to fit the model. Due to recent developments in computational power and optimization algorithms, NMPC techniques are becoming increasingly accepted in the chemical industries, NMPC being one of the approaches, which inherently can cope with process constraints, nonlinearities, and different objectives derived from economical or environmental considerations. In this paper an efficient real-time NMPC is applied to an industrial pilot batch polymerization reactor. The approach exploits the advantages of an efficient optimization algorithm based on multiple shooting technique [FAww], [Die01] to achieve real-time feasibility of the on-line optimization problem, even in the case of the large control and prediction horizons. The NMPC is used for tight setpoint tracking of the optimal temperature profile. Based on the available measurements the complex model is not observable hence cannot be used directly in the NMPC strategy. To overcome the problem of unobservable states, a grey-box modelling approach is used, where some unobservable parts of the model are described through nonlinear empirical relations, developed from the detailed first-principles model. The resulting control-relevant model is fine tuned using experimental data and maximum likelihood estimation. A parameter adaptive extended Kalman filter (PAEKF) is used for state estimation and on-line parameter adaptation to account for model/plant mismatch.

## 2 Nonlinear Model Predictive Control

### 2.1 Algorithm Formulation

Nonlinear model predictive control is an optimization-based multivariable constrained control technique that uses a nonlinear dynamic model for the prediction of the process outputs. At each sampling time the model is updated on the basis of new measurements and state variable estimates. Then the open-loop optimal manipulated variable moves are calculated over a finite prediction horizon with respect to some cost function, and the manipulated variables for the subsequent prediction horizon are implemented. Then the prediction horizon is shifted or shrunk by usually one sampling time into the future and the previous steps are repeated. The optimal control problem to be solved on-line in every sampling time in the NMPC algorithm can be formulated as:

$$\min_{u(t)\in\mathcal{U}} \{\mathcal{H}(x(t),u(t);\theta) = \mathcal{M}(x(t_F);\,\theta) + \int_{t_k}^{t_F} \mathcal{L}(x(t),u(t);\theta)dt\} \tag{1}$$

$$s.t.\;\; \dot{x}(t) = f(x(t),\; u(t);\; \theta), \qquad x(t_k) = \hat{x}(t_k), \quad x(t_0) = \hat{x}_0 \tag{2}$$

$$h(x(t),\; u(t);\; \theta) \leq 0, \qquad t \in [t_k,\; t_F] \tag{3}$$

where $\mathcal{H}$ is the performance objective, $t$ is the time, $t_k$ is the time at sampling instance $k$, $t_F$ is the final time at the end of prediction, is the $n_x$ vector of states, $u(t) \in \mathcal{U}$ is the $n_u$ set of input vectors, is the $n_y$ vector of measured variables used to compute the estimated states $\hat{x}(t_k)$, and $\theta \in \Theta \subset \mathcal{R}^{n_\theta}$ is the $n_\theta$ vector of possible uncertain parameters, where the set $\Theta$ can be either defined by hard bounds or probabilistic, characterized by a multivariate probability density function. The function $f : \mathcal{R}^{n_x} \times \mathcal{U} \times \Theta \rightarrow \mathcal{R}^{n_x}$ is the twice continuously differentiable vector function of the dynamic equations of the system, and $h : \mathcal{R}^{n_x} \times \mathcal{U} \times \Theta \rightarrow \mathcal{R}^c$ is the vector of functions that describe all linear and nonlinear, time-varying or end-time algebraic constraints for the system, where $c$ denotes the number of these constraints.

We assume that $\mathcal{H} : \mathcal{R}^{n_x} \times \mathcal{U} \times \Theta \rightarrow \mathcal{R}$ is twice continuously differentiable, thus fast optimization algorithms, based on first and second order derivatives may be exploited in the solution of (1). The form of $\mathcal{H}$ is general enough to express a wide range of objectives encountered in NMPC applications. In NMPC the optimization problem (1)-(3) is solved iteratively on-line, in a moving (receding) horizon ($t_F < t_f$) or shrinking horizon ($t_F = t_f$) approach, where $t_f$ is the batch time.

### 2.2 Solution Strategy and Software Tool

Considering the discrete nature of the on-line control problem, the continuous time optimization problem involved in the NMPC formulation is solved by formulating a discrete approximation to it, that can be handled by conventional nonlinear programming (NLP) solvers [BR91], [Bie00]. The time horizon $t \in [t_0,\ t_f]$ is divided into $N$ equally spaced time intervals $\Delta t$ (stages), with discrete time steps $t_k = t_0 + k\Delta t$, and $k = 0, 1, ..., N$. Model equations are discretized, $x_{k+1} = f_k(x_k, u_k; \theta)$, and added to the optimization problem as constraints. For the solution of the optimization problem a specially tailored NMPC tool (*OptCon*) was developed that includes a number of desirable features. In particular, the NMPC is based on first-principles or grey box models, and the problem setup can be done in Matlab. The NMPC approach is based on a large-scale NLP solver (HQP) [FAww], which offers an efficient optimization environment, based on multiple shooting algorithm, that devides the optimization horizon into a number of subintervals (stages) with local control parameterizations. The differential equations and cost on these intervals are integrated independently during each optimization iteration, based on the current guess of the control. The continuity/consistency of the final state trajectory at the end of the optimization is enforced by adding consistency constraints to the nonlinear programming problem.

### 2.3 Real-Time Implementation

In NMPC simulation studies usually immediate feedback is considered, i.e. the optimal feedback control corresponding to the information available up to the moment $t_k$, is computed, $u^\star(t_k) = [u_{0|t_k}, u_{1|t_k}, \ldots, u_{N|t_k}]$, and the first value ($u_{0|t_k}$)

is introduced into the process considering no delay. However, the solution of the NLP problem requires a certain, usually not negligible, amount of computation time $\delta_k$, while the system will evolve to a different state, where the solution $u^\star(t_k)$ will no longer be optimal [FA02]. Computational delay $\delta_k$ has to be taken into consideration in real-time applications. In the approach used here, in moment $t_k$, first the control input from the second stage of the previous optimization problem $u_{1|t_{k-1}}$ is injected into the process, and then the solution of the current optimization problem is started, with fixed $u_{0|t_k} = u_{1|t_{k-1}}$. After completion, the optimization idles for the remaining period of $t \in (t_k + \delta_k, t_{k+1})$, and then at the beginning of the next stage, at moment $t_{k+1} = t_k + \Delta t$ , $u_{1|t_k}$ is introduced into the process, and the algorithm is repeated. This approach requires real-time feasibility for the solution of each open-loop optimization problems ($\delta_k \leq \Delta t$).

### 2.4 State Estimation

Proper state estimation is crucial for successful practical NMPC applications. Extended Kalman filter (EKF) is widely used in process control applications, however its performance strongly depends on the accuracy of the model. To avoid highly biased model predictions, selected model parameters are estimated together with the states, leading to a parameter adaptive EKF formulation [VG00]. Define $\theta' \subseteq \theta$ as the vector of the estimated parameters from the parameter vector, and $\theta'' \triangleq \theta \backslash \theta'$ the vector of the remaining parameters. The augmented state vector in this case is given by $\mathcal{X} = [x,\ \theta']^T$, and the augmented model used for estimation is, $\dot{\mathcal{X}} = [f(x,\ \theta', u;\ \theta''),\ \mathbf{0}]^T + [w,\ \ w_{\theta'}]^T$, with $w$ , and $w_{\theta'}$ zero-mean Gaussian white noise variables. The measurement covariance matrix is determined based on the accuracy of the measurements. The appropriate choice of the state covariance matrix, $\mathbf{Q}$, is however often difficult in practical applications. An estimate of $\mathbf{Q}$ can be obtained by assuming that the process noise vector mostly represents the effects of parametric uncertainty [VG00], [NB03]. Based on this assumption the process noise covariance matrix can be computed as $\mathbf{Q}(t) = \mathbf{S}_\theta(t)\mathbf{V}_\theta\mathbf{S}_\theta^T(t)$, with $\mathbf{V}_\theta \in \mathcal{R}^{n_\theta \times n_\theta}$ being the parameter covariance matrix, and $\mathbf{S}_\theta(t) = (\partial f/\partial\theta)_{\hat{x}(t),u(t),\hat{\theta}}$ is the sensitivity jacobian computed using the nominal parameters and estimated states. This approach provides an easily implementable way to estimate the process noise covariance matrix, since the parameter covariance matrix $\mathbf{V}_\theta$ is usually available from parameter estimation, and the sensitivity coefficients in $\mathbf{S}_\theta$ can be computed by finite differences or via sensitivity equations. Note that the above approach leads to a time-varying, full covariance matrix, which has been shown to provide better estimation performance for batch processes than the classically used constant, diagonal $\mathbf{Q}$ [VG00], [NB03].

## 3 Practical Implementation of NMPC to an Industrial Pilot Batch Reactor

A schematic representation of the experimental pilot plant is shown on Figure 1. The reactor temperature is controlled using a complex heating-cooling system, which is based on a closed oil circuit, which is recycled through the jacket with a constant flow rate $F_j$. The heating-cooling medium goes through a multi-tubular heat exchanger where a PI controller is used to keep the temperature difference constant, by adjusting the cooling water flow rate. Heating is performed using an electric heater. The power of the heater is adjusted by a PI controller that regulates the input temperature into the jacket. The setpoint of the PI controller is determined by the higher level NMPC that has the objective to track a predetermined temperature profile in the reactor.

A detailed first-principles model of the process containing material and energy balances as well as detailed kinetic and thermodynamic models was used and identified based on off-line experiments. Since only temperature measurements are available in the plant, many states of the detailed model are not estimable, or not even detectable. The complex model however was used to determine the optimal temperature profile, and for deriving the control-relevant model. Available measurements are: reactor temperature ($T_r$), and input and output temperatures into and from the jacket, ($T_{jin}$, $T_j$). With this set of measurements the following reduced model was used in the NMPC:

$$\dot{n}_M = -Q_r/\Delta H_r \tag{4}$$

$$\dot{T}_{r,k} = \frac{Q_r + U_w A_w (T_{w,k} - T_{r,k}) - (UA)_{loss,r}(T_{r,k} - T_{amb})}{m_M c_{p,M} + m_P c_{p,P} + m_{water} c_{p,water}} \tag{5}$$

$$\dot{T}_{w,k} = (U_j A_j (T_{j,k} - T_{w,k}) - U_w A_w (T_{w,k} - T_{r,k}))/m_w/c_{pw} \tag{6}$$

$$\dot{T}_{j,k} = \frac{\mathcal{N} F_j \rho_j c_{p,j} (T_{j,k-1} - T_{j,k}) - U_j A_j (T_{j,k} - T_{w,k}) - (UA)_{loss,j}(T_{j,k} - T_{amb})}{m_j c_{p,j}} \tag{7}$$

where $k = 1, \ldots, \mathcal{N}$, $T_r = T_{r,\mathcal{N}}$, $T_j = T_{j,\mathcal{N}}$, $T_{j,0} = T_{jin}$, $n_M$ is the number of mol of monomer, $\Delta H_r$ is the enthalpy of reaction, $T_w$ is the wall temperature, $U$ and $A$ are heat transfer coefficients and areas from reactor to wall $(\cdot)_w$ or wall to jacket $(\cdot)_j$, $c_{p,M/P/water/w/j}$ and $m_{M/P/water/w/j}$ are the heat capacities and masses of monomer, polymer, water, wall and oil, $T_{amb}$ is the ambient temperature, $\rho_j$ is the density of the oil, $(UA)_{loss,r/j}$ heat loss coefficients in the reactor and jacket, respectively.

To estimate the transport delay, the reactor, wall and jacket were divided in $\mathcal{N} = 4$ elements, leading to a system of 13 differential equations. To achieve proper prediction and maintain the observability of the model, with only temperature measurements available, different approaches have been proposed. Helbig et al. used a time series of the estimated heat generation determined from simulation of a batch [HA96]. The industrial batch MPC product developed by IPCOS determines an empirical nonlinear relation $Q_r = f_Q(n_M, T_r)$, which expresses the heat generation as a function of the conversion and temperature [IP00]. In our case study a similar approach was used. The empirical nonlinear relation was determined from the complex first principle model, simulating the process for different temperature profiles.

Maximum likelihood estimation was used to fit the parameters of the model (4)-(7) to the data obtained from the plant, performing several water batches (when $Q_r = 0$), using $\theta'' = [(UA)_{loss,r},\ (UA)_{loss,j},\ U_jA_j,\ m_w,\ m_j]$ as the parameter vector. This procedure gives the optimal nominal parameter estimates, $\hat{\theta''}^{\star}$, and the corresponding uncertainty description given by the covariance matrix, estimated from the Hessian of the objective used in the maximum likelihood estimation. The good fit between the experimental data and the model is shown on Figure 2.

Model (4)-(7) was used in an adaptive output feedback NMPC approach, where the objective was to provide a tight setpoint tracking, by minimizing online, in every sampling instance $k$, the following quadratic objective:

$$\min_{u(t)} \int_{t_k}^{t_F} \{(T_r(t) - T_r^{ref}(t))^2 + Q_{\Delta u}(du(t))^2\}dt \qquad (8)$$

The optimal setpoint profile $T_r^{ref}$ is generally obtained via off-line optimization using the detailed model. In our implementation however, a suboptimal but typical profile consisting of three piece-wise linear segments was used. The manipulated input of the NMPC, $u(t) = T_{jSP}$, is the setpoint temperature

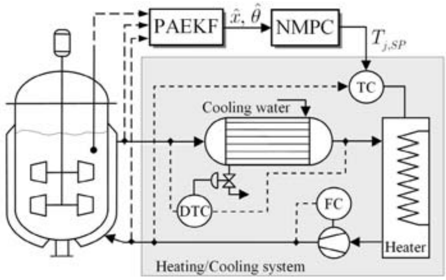


**Fig. 1.** Schematic representation of the batch reactor system

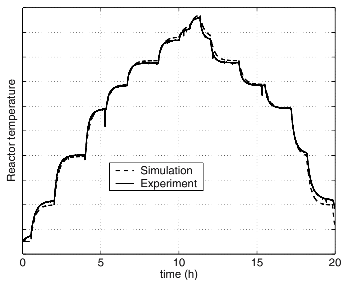


**Fig. 2.** Validation of the model compared to plant data

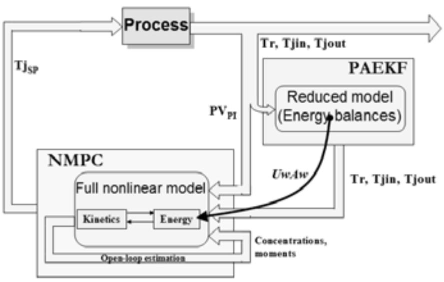


**Fig. 3.** Implementation structure of the PAEKF and NMPC

to the lower level PI controller, which controls the jacket input temperature. The communication between the real plant and NMPC was performed via the standard OPC interface. The adaptive structure of the implemented NMPC is shown on Figure 3. During the batch the heat transfer properties in the reactor change significantly thus the adaptive algorithm is important. The parameters $\theta' = [Q_r,\ U_w A_w]$ were estimated together with the model states in the PAEKF. Figure 4 indicates a strong variation of $U_w A_w$ during the batch. Figure 5 demonstrates the very good setpoint tracking performance of the NMPC with adapted model. The parameter covariance matrix $\mathbf{V}_\theta$, resulted from the identification was used to compute the state covariance matrix in the estimator [VG00], [NB03]. A weighting coefficient of $Q_{\Delta u} = 0.4$, and prediction and control horizons of $8000s$ were used, in the optimization, with a sampling time of $20s$. The control input was discretized in 400 piecewise constant inputs, leading to a high dimensional optimization problem. The efficient multiple shooting approach guarantees the real-time feasibility of the NMPC implementation. Even with the large control discretization of 400 the computation time was below the sampling time of $20s$ (approx. $5s$). All simulation times are on a Pentium 3, 800 MHz PC running Windows 2000.

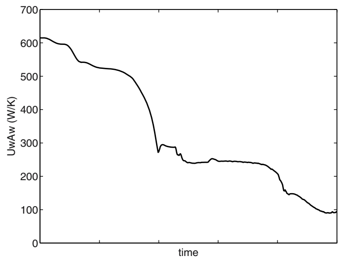


**Fig. 4.** Estimated Heat transfer coefficient during the batch

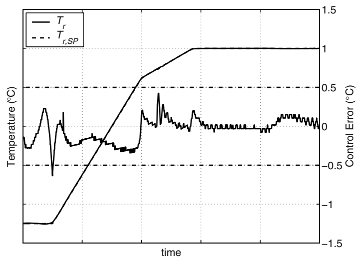


**Fig. 5.** Experimental results: NMPC of the industrial batch reactor

## 4 Conclusions

The paper present a computationally efficient NMPC approach that combines output feedback design with efficient optimization technique providing a framework that can be supported in an industrial environment. Detailed first-principles model is used to derive the reduced control-relevant model based on the available measurements, which is tuned using data from the plant, and used then in the NMPC. A PAEKF is combined with the control algorithm for the on-line state estimation and model adaptation to achieve offset free control. Simulation and experimental results demonstrate the efficiency of the NMPC approach in an industrial application.

## References


[Die01] Diehl, M.: Real-Time Optimization for Large Scale Nonlinear Processes. PhD Thesis, University of Heidelberg, Heidelberg (2001)

[Bie00] Biegler, L.: Efficient solution of dynamic optimization and NMPC problems. In: F. Allgoewer and A. Zheng, (eds), Nonlinear Predictive Control. Birkhauser, Bagel (2000)

[QB03] Qin S.J., Badgwell, T.: A Survey of Industrial Model Predictive Control Technology. Control Engineering Practice, **11**, 733–764 (2003)

[ML97] Morari, M., Lee, J.H.: Model predictive control: Past, present and future. In Proc. PSE'97-ESCAPE-7 Symposium, Trondheim, (1997)

[Hen98] Henson, A.M.: Nonlinear model predictive control: current status and future directions. Comp. Chem. Eng., **23**, 187–201 (1998)

[FA02] Findeisen, R., Allgoewer, F.: Nonlinear model predictive control: From theory to application. In Int. Symp. on Design, Operation and Control of Chemical Plants (PSE Asia'02), Taipei, Taiwan (2002)

[FAww] Franke, R., Arnold, E. Linke H.: HQP: A solver for nonlinearly constrained large-scale optimization. http://hqp.sourceforge.net

[BR91] Biegler, L.T., Rawlings, J.B.: Optimisation approaches to nonlinear model predictive control. Proceedings of Conf. Chemical Process Control, South Padre Island, Texas, 543–571 (1991)

[VG00] Valappil, J., Georgakis, C.: Systematic estimation of state noise statistics for Extended Kalman Filters. AIChE J., **46**, 292–308 (2000)

[NB03] Nagy, Z.K., Braatz, R.D.: Robust nonlinear model predictive control of batch processes. AIChE J., **49**, 1776–1786 (2003)

[HA96] Helbig, A., Abel, O., M'hamdi, A., Marquardt, W.: Analysis and nonlinear model predictive control of the Chylla-Haase Benchmark problem. Proceedings of UKACC International Conf. on Control 1172–1177 (1996)

[IP00] Van Overschee, P., Van Brempt, W.: polyPROMS IPCOS-ISMC Final Report, Internal Report of the polyPROMS European 5th Framework Research Project GRD1-2000-25555.