

Nonlinear Model Predictive Control Using Successive Linearization - Application to Chemical Reactors -

Hiroya SEKI*, Satoshi OYAMA** and Morimasa OGAWA***

A nonlinear model predictive control based on successive linearization approach is developed. A nonlinear process model is linearized along its trajectory and an infinite-time horizon linear optimal regulator with integrator is implemented in a receding horizon fashion. Simulation examples for highly nonlinear chemical reactors which exhibit static input or output multiplicities are given to demonstrate the capability of the controller. The developed control algorithm has been successfully applied to a grade transition operation in an industrial polymerization reactor.

Key Words: Process control, nonlinear control, model predictive control, chemical reactor, industrial application

1. Introduction

Model predictive control (MPC), which was originally developed in the 1970's to meet the specialized control needs of power plants and petroleum refineries, can now be found in a wide variety of application areas especially in the petroleum and petrochemical industries¹⁾. However, most of industrial applications are limited to linear MPC (LMPC), in which controlled plants are weakly nonlinear or operating regions are limited so that the assumptions of linearity may hold.

Representative of highly nonlinear chemical processes to which LMPC applications are difficult, are chemical reactors, the core of a chemical process. Among the nonlinearities exhibited by chemical reactors, steady state input multiplicities^{2), 3)} and output multiplicities^{4)~7)} can be cited as detrimental to feedback control. With nonlinear processes which exhibit output multiplicities, there exist more than one set of outputs for a certain set of inputs in their steady state relations; in most cases, they are accompanied by changes in open-loop stability. On the other hands, with processes exhibiting input multiplicities, there exist more than one set of inputs for a certain set of outputs; this implies that the sign of the steady state gain (in the case of multivariable systems, the sign of the determinant of the steady state gain matrix) changes in the operating region, and there may exist sets of setpoints which are unreachable.

For these kinds of nonlinear processes, it would be difficult to cover a wide range of operating conditions with a single linear controller. Especially for processes with input multiplicities, a linear controller with integral action necessarily becomes unstable if a sign change in the steady state gain occurs⁸⁾.

Nonlinear MPC (NMPC), which employs a nonlinear process model to predict future process responses and calculate manipulated variable moves, possesses a strong potentiality of improving control and operation of nonlinear processes. The underlying principle of NMPC is the same as that of LMPC with the exception that the model describing the process dynamics is nonlinear. However, from implementation viewpoints, it poses some technical problems, which are associated with computational burdens⁹⁾; even with the currently available CPU power, application of NMPC, in which a nonlinear optimization problem has to be solved on-line, requires formidable efforts in order to calculate control actions within fixed sampling time. NMPC based on successive linearization^{10), 11)}, which uses a locally linearized model at each control interval, is currently the most practical and promising technique for industrial applications.

In this paper, NMPC algorithm using the successive linearization approach is first described. Motivated by the fact that unconstrained LMPC with infinite-time prediction/control horizons is known to be equivalent to linear quadratic regulator (LQR) and nice stability property is guaranteed, we apply LQR control problem to the locally linearized process model successively obtained at each control sampling time. Particular attention is paid to the solvability of the LQR problem, in which singularity of the steady state gain matrix becomes a critical issue.

* Formerly at Mitsubishi Chemical Corp. Current affiliation: Chemical Resources Laboratory, Tokyo Institute of Technology

** Mitsubishi Chemical Corp.

*** Formerly at Mitsubishi Chemical Corp. Current affiliation: Yamatake Corp. Advanced Automation Company

Secondly, simulation studies are performed using nonlinear chemical reactor examples which exhibit input or output multiplicities. Finally, application to grade transition operations of an industrial high density polyethylene (HDPE) polymerization reactor is presented.

2. Nonlinear MPC using successive linearization

A process is assumed to be described by the following nonlinear ordinary differential equation:

$$\dot{x} = f(x, u), \quad (1)$$

$$y = h(x), \quad (2)$$

where $x \in \mathfrak{R}^n$, $u, y \in \mathfrak{R}^m$ are a state variable, a manipulated variable and a controlled variable respectively.

We assume that the process is square and we design a controller which realizes offset free responses of the controlled variable y to its target value $r(t) \in \mathfrak{R}^m$.

2.1 Control algorithm

Defining the values of each variable at time $t = t_k$ as $x_k = x(t_k)$, $u_k = u(t_k)$, $y_k = y(t_k)$, the control algorithm is described as follows. The algorithm is presented here in the continuous time domain for brevity, but in practice it would be implemented in discrete time.

Step 1 (Local linearization) Around the current trajectory (x_k, u_k) , the process model (1)(2) is linearized:

$$\Delta \dot{x}_k = A_k \Delta x_k + B_k \Delta u_k + \delta_k \quad (3)$$

$$\Delta y_k = C_k \Delta x_k, \quad (4)$$

where

$$\Delta x_k = x(t) - x_k, \Delta u_k = u(t) - u_k, \Delta y_k = y(t) - y_k,$$

$$A_k = \frac{\partial f}{\partial x}(x_k, u_k), \quad B_k = \frac{\partial f}{\partial u}(x_k, u_k),$$

$$C_k = \frac{\partial h}{\partial x}(x_k, u_k), \quad \delta_k = f(x_k, u_k).$$

The following assumption is made:

Assumption 1. The locally linearized system (3)(4) is stabilizable and detectable.

Step 2 (Determination of steady state target by the least squares method) Steady state target \bar{x}_k, \bar{u}_k is obtained as the solution to the following least squares problem:

$$\min_{\Delta x_k, \Delta u_k} J = (\Delta r_k - C_k \Delta x_k)^T (\Delta r_k - C_k \Delta x_k) + \Delta u_k^T R_1 \Delta u_k \quad (5)$$

subject to

$$A_k \Delta x_k + B_k \Delta u_k + \delta_k = 0, \quad (6)$$

where $\Delta r_k = r(t_k) - y_k$, and $R_1 \in \mathfrak{R}^{m \times m}$ is a positive definite tuning weight matrix.

The least squares solution is given as

$$\begin{pmatrix} \bar{x}_k \\ \bar{u}_k \\ \lambda \end{pmatrix} = \begin{pmatrix} C_k^T C_k & O & A_k^T \\ O & R_1 & B_k^T \\ A_k & B_k & O \end{pmatrix}^{-1} \begin{pmatrix} C_k^T \Delta r_k \\ 0 \\ -\delta_k \end{pmatrix}, \quad (7)$$

where $\lambda \in \mathfrak{R}^n$ is a Lagrange multiplier.

Step 3 (LQ control problem) The locally linearized model is augmented with integrators at input, and the linear optimal regulator is constructed around the steady state target obtained at Step 2. If we define

$$z_k = \begin{pmatrix} \Delta x_k - \bar{x}_k \\ \Delta u_k - \bar{u}_k \end{pmatrix}, \quad v_k = \Delta \dot{u}_k, \quad (8)$$

$$F_k = \begin{pmatrix} A_k & B_k \\ O_{m \times n} & O_{m \times m} \end{pmatrix}, \quad G_k = \begin{pmatrix} O_{n \times m} \\ I_m \end{pmatrix},$$

the augmented system can be described as

$$\dot{z}_k = F_k z_k + G_k v_k, \quad z_k(t_k) = \begin{pmatrix} -\bar{x}_k \\ -\bar{u}_k \end{pmatrix}, \quad (9)$$

where I_m is the m -th order identity matrix.

To the above system, the infinite-time horizon LQ control problem is applied:

$$\min_{v_k} J_k = \int_{t_k}^{\infty} \{z_k^T Q_k z_k + v_k^T R_2 v_k\} dt, \quad (10)$$

where

$$Q_k = \begin{pmatrix} C_k^T C_k & O \\ O & R_1 \end{pmatrix}, \quad Q_k \in \mathfrak{R}^{(n+m) \times (n+m)}. \quad (11)$$

The matrix $R_2 \in \mathfrak{R}^{m \times m}$ is a positive definite weight matrix and used as tuning parameter.

The solution to the optimal control problem v_k^* is obtained by solving the associated Riccati equation as

$$\dot{v}_k^*(t) = -K_k z_k(t), \quad (12)$$

where $K_k \in \mathfrak{R}^{m \times (n+m)}$ is the regulator gain matrix.

Step 4 (Implementation of control input) The initial value of the optimal control input obtained at Step 3:

$$v_k^*(t_k) = -K_k z(t_k) = K_k \begin{pmatrix} \bar{x}_k \\ \bar{u}_k \end{pmatrix} \quad (13)$$

is implemented on the plant.

2.2 Characteristics of the control algorithm

When constructing a linear servo system for a constant setpoint, it is assumed that the following matrix is nonsingular¹²⁾:

$$\Phi_k = \begin{pmatrix} A_k & B_k \\ C_k & O \end{pmatrix}. \quad (14)$$

However, with nonlinear systems which exhibit input multiplicities, the matrix Φ_k may become singular. Also with general nonlinear systems, nonsingularity of the matrix Φ_k may not be guaranteed along all the trajectories. For

a linear system with singular Φ_k , a linear optimal regulator cannot be constructed because steady state for a given setpoint r is not uniquely determined. In order to solve this problem, weighting R_1 on the input Δu_k is introduced to the least squares problem (5) and the steady state target is updated at each control sampling time; existence of the inverse matrix in Equation (7) is guaranteed if the assumption 1 and $R_1 > 0$ hold. Note that the LQR problem (10) is also solvable. For general nonlinear systems with which the assumption 1 does not hold, the control algorithm is not applicable.

For linear systems, model predictive control with infinite-time prediction/control horizons is known to be equivalent to LQR. However, the control algorithm presented here differs from LQR because the steady state target is updated at each control interval due to the weight R_1 (if $R_1 = 0$, it coincides with the LQR). However, nominal closed loop stability can be proven¹³).

The reason why the process is augmented at its input is the industrial requirements that aggressive input variable changes are not desired most often and offset free steady state responses are preferred.

Through rearrangement of equations, the controller can be described in the following form:

$$\dot{u} = K_1 \{r - h(x)\} + K_2 f(x, u), \quad (15)$$

where

$$K_1 = R_2^{-1} G^T (F - GK)^{-T} [C \ O_{m \times m}]^T, \quad (16)$$

$$K_2 = -R_2^{-1} G^T (F - GK)^{-T} P_1, \quad (17)$$

and $P_1 \in \mathfrak{R}^{(n+m) \times n}$ is a submatrix defined for the unique solution $P \in \mathfrak{R}^{(n+m) \times (n+m)}$ of the Riccati equation and defined by

$$\begin{pmatrix} P_1 & P_2 \end{pmatrix} = P. \quad (18)$$

In Eqs (15)-(18), the matrices are the same as those defined in the previous subsection (subscript k is omitted) and they are functions of (x, u) .

The closed loop has the following steady state properties:

Reachable setpoint: When the matrix Φ evaluated at the equilibrium corresponding to the given setpoint is nonsingular, it can be shown that $\det K_1 \neq 0$. At equilibrium, $f(\cdot) = 0$ holds, so that Eq. (15) implies $r = h(x)$ is the unique solution which makes $\dot{u} = 0$. That is, there exists no steady state error. However, in an actual process with modeling errors, $f(\cdot) = 0$ of the model does not necessarily hold at the true process equilibrium, so that steady state error may exist; this is a consequence of augmenting the plant at its *input*,

not directly integrating the error between the setpoint and the controlled variable. The method for eliminating steady state errors is described in the next section.

Unreachable setpoint: With nonlinear processes which exhibit input multiplicities, there may be cases where given setpoints are unreachable (a linear controller surely becomes unstable). In this case, the closed loop converges to an equilibrium where $\det \Phi = 0$ and the steady state error belongs to the null space of K_1^T (in the case $\det \Phi = 0$, it results in $\det K_1 = 0$)¹³).

2.3 State estimation and steady state properties of the closed loop

In the previous section, it is assumed that the state variable is known, but practically we have to estimate them in some way. Also, offset free estimation of the controlled variables is required to construct a closed loop which realizes offset free response to a constant setpoint.

Here, we introduce steady state extended Kalman filter which assumes a constant disturbance at its input.

State estimator with input disturbance The process model is augmented as follows:

$$\begin{aligned} \dot{\hat{x}} &= f(\hat{x}, u + \xi) \\ \dot{\hat{\xi}} &= 0 \\ \hat{y} &= h(\hat{x}), \end{aligned} \quad (19)$$

where $\hat{x} \in \mathfrak{R}^n$, $\hat{y} \in \mathfrak{R}^m$ and $\xi \in \mathfrak{R}^m$ are the estimate of state variable, output variable and input disturbance, respectively.

At time $t = t_k$, steady state Kalman filter is constructed for the matrix pair:

$$\begin{pmatrix} A_k & B_k \\ O_{m \times n} & O_{m \times m} \end{pmatrix}, \begin{pmatrix} C_k & O_{m \times m} \end{pmatrix}. \quad (20)$$

The dynamics of the state estimator is described as

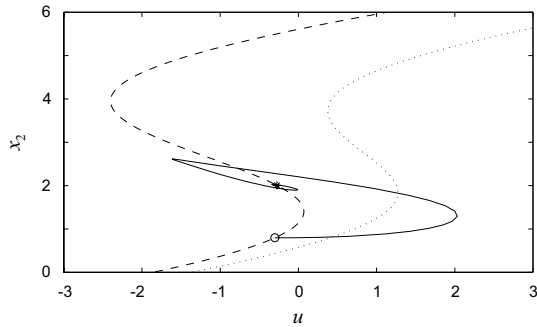
$$\begin{aligned} \dot{\hat{x}} &= f(\hat{x}, u + \xi) + K_{\hat{x}}(y - \hat{y}) \\ \dot{\hat{\xi}} &= K_{\hat{\xi}}(y - \hat{y}) \\ \hat{y} &= h(\hat{x}), \end{aligned} \quad (21)$$

where $K_{\hat{x}} \in \mathfrak{R}^{n \times m}$ and $K_{\hat{\xi}} \in \mathfrak{R}^{m \times m}$ are the submatrix of the Kalman filter gain matrix.

If the matrix pair (20) is detectable and the Kalman filter gain matrix is obtained, we can prove that the submatrix $K_{\hat{\xi}}$ is nonsingular, so that Eq. (21) implies that $y = \hat{y}$, $f(\cdot) = 0$ for the steady state ($\dot{\hat{x}} = 0$, $\dot{\hat{\xi}} = 0$), resulting in offset free estimation of the output. Moreover, Eq. (15) implies that if the closed loop is stable, it achieves an offset free response to a constant setpoint regardless of model errors.

Table 1 Process and model parameters for the CSTR with output multiplicities

	τ	γ	D_a	λ	β	x_{10}	x_{20}
process	1.0	40.0	0.075	-8.0	0.3	1.0	1.0
model	1.0	40.0	0.0675	-7.2	0.33	1.0	1.0

**Fig. 1** Closed loop response of the CSTR with output multiplicities. The dashed and dotted lines are the steady state input/output relation of the process and the model, respectively. The point marked by 'o' is the initial condition and '*' is the set-point.

3. Simulations

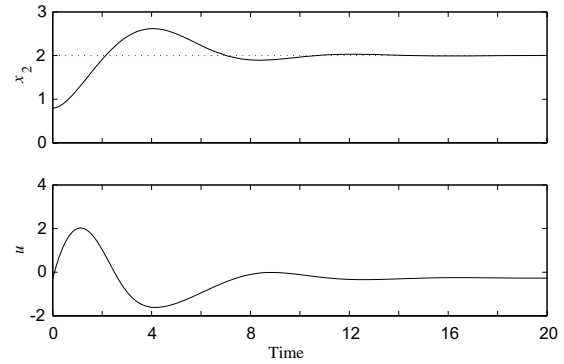
3.1 Chemical reactor with output multiplicities⁶⁾

The example process is a continuous stirred tank reactor (CSTR) with a cooling jacket, in which the 1st order exothermic reaction $A \rightarrow B$ occurs. The process model is described as follows:

$$\begin{aligned} \tau \dot{x}_1 &= (-x_1 + x_{10}) - D_a \exp\left(\frac{x_2}{1 + x_2/\gamma}\right) x_1 \\ \tau \dot{x}_2 &= (-x_2 + x_{20}) + \lambda D_a \exp\left(\frac{x_2}{1 + x_2/\gamma}\right) x_1 \\ &\quad - \beta(x_2 - u) \\ y &= x_2, \end{aligned} \quad (22)$$

where x_1, x_2 and u are normalized concentration of A, reactor temperature and jacket temperature respectively. The model parameters are listed in **Table 1**, together with the model errors assumed in the simulation calculation. This process exhibits steady state output multiplicities and open loop stability property changes depending on operating points.

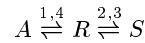
Figs. 1, 2 show the closed loop responses to a setpoint $r = 2.0$ with the initial condition $(x_1, x_2) = (0.8593, 0.7966)$, $u = -0.301$. The tuning parameters are $R_1 = 1.0 \times 10^{-2}$, $R_2 = 1.0 \times 10^{-1}$. In this example, the process is controlled from an open loop stable equilibrium to an open loop unstable equilibrium. The closed loop converges to the setpoint without steady state errors even under the presence of the modeling errors.

**Fig. 2** Closed loop response of the CSTR with output multiplicities. The dotted line is the set-point.**Table 2** Model parameters for the CSTR with input multiplicities

i	1	2	3	4
k_{i0}	1.0	0.7	0.1	0.006
E_i/RT_0	8.33	10	50	83.3

3.2 Chemical reactor with input multiplicities⁴⁾

The next example process is a CSTR with the reaction:



and its dynamics is described by

$$\begin{aligned} \dot{c}_A &= u_1(c_{A0} - c_A) - k_1 c_A + k_4 c_R \\ \dot{c}_R &= u_1(1 - c_{A0} - c_R) + k_1 c_A + k_3(1 - c_A - c_R) \\ &\quad - (k_2 + k_4) c_R \\ y &= \begin{pmatrix} c_A & c_R \end{pmatrix}^T, \end{aligned} \quad (23)$$

where c_i ($i = A, R$) is the concentration of each species, c_{A0} is the concentration of A in the feed, u_1 is the feed rate, u_2 is the reaction temperature. All the variables are normalized. The reaction rate constants $k_1 \sim k_4$ are expressed in the Arrhenius form:

$$k_i = k_{i,0} \exp\left[-\frac{E_i}{RT_0} \left(\frac{1}{u_2} - 1\right)\right]. \quad (24)$$

Model parameters are listed in **Table 2**.

This process exhibits steady state input multiplicities, and the determinant of the gain matrix from the input $u = (u_1 \ u_2)^T$ to $y = (c_A \ c_R)^T$ changes sign. There are unreachable setpoints.

Figs. 3, 4 show the closed loop response to a setpoint $r = (0.28 \ 0.28)^T$ with the initial condition $(c_A, c_R) = (0.2989, 0.3596)$, $(u_1, u_2) = (0.2083, 0.8879)$ and $c_{A0} = 0.8$. The state variables c_A, c_R are both measured and $R_1 = 10^{-2} I_2, R_2 = 10^{-3} I_2$. In the $u_1 - u_2$ plot of Fig. 3, $+-$ denote the sign of the determinant of the steady state gain matrix at that point. The given setpoint r is unreachable at steady states (it is in the region marked by 'Unreachable' in $c_A - c_R$ plot of Fig. 3), but the closed

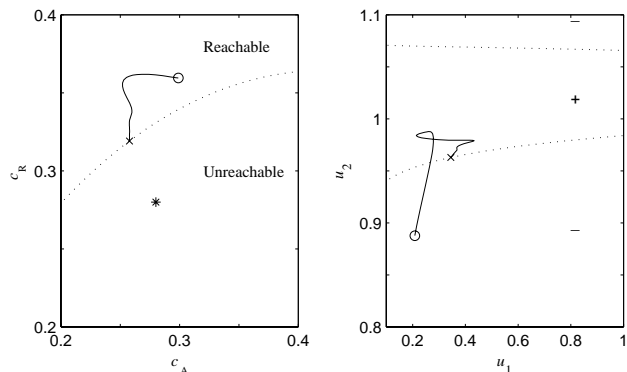


Fig. 3 Closed loop response of the CSTR with input multiplicities. The dotted lines are the loci along which the steady state gain matrix becomes singular. The points marked by 'o' are the initial conditions, and 'x' are the final states, and '*' are the set-points.

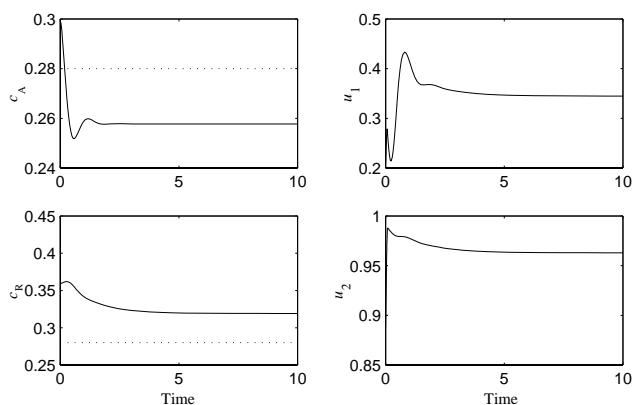


Fig. 4 Closed loop response of the CSTR with input multiplicities. The dotted lines are the set-points.

loop converges to a point where the determinant of the steady state gain matrix is zero. As shown in this example, the closed loop remains stable even for an unreachable setpoint.

4. Industrial application

The control algorithm is applied to a polymerization reactor for HDPE (High Density Polyethylene) production. The reactor does not exhibit input or output multiplicities, but its frequent grade changeover operations require control systems to cover a wide operating range; in the conventional reactor operations, a linear control system has been utilized, but controlled responses during grade transition are rather sluggish so that there are frequent operator interventions.

Fig. 5 shows the process flow diagram. Gaseous monomer (ethylene), comonomer (propylene), and hydrogen are fed to the reactor together with catalysts. These feed streams are controlled by PID controllers. The prod-

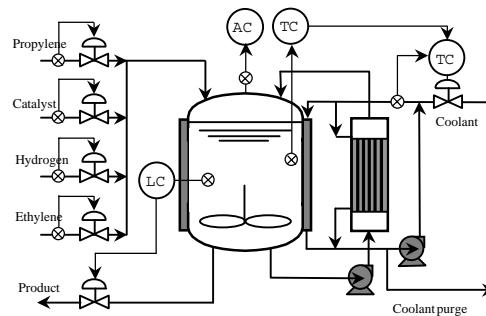


Fig. 5 Process flow of the HDPE reactor.

uct flow of polyethylene is used to control the reactor slurry level. The reactor temperature is controlled by the cooling jacket and the recycle cooler. The reactor pressure and gas compositions are available for the feedback control.

A basic operation of the process is to adjust the partial pressure of each gas composition (more precisely, the reactor pressure, the ratio of hydrogen/ethylene, and propylene/ethylene in the gas phase which are strongly related to the key polymer properties such as Melt Index and density) to specified values, which are determined in accordance with a polymer grade being produced, by manipulating the feed gas streams. The set-point in the reactor temperature is also determined according to polymer grades. The set-point in the production rate is changed by market demand.

In the conventional linear control system, multi-loop LMPC has been utilized with the pairings: production rate ↔ monomer feed rate, monomer partial pressure ↔ catalyst feed rate, hydrogen/monomer partial pressure ratio ↔ hydrogen feed rate, comonomer/monomer partial pressure ratio ↔ comonomer feed rate.

In designing NMPC, a fourth order process model which describes the mass balance for the monomer, hydrogen, comonomer and catalyst is developed¹⁴⁾. The controlled variables are selected as the monomer partial pressure, the hydrogen partial pressure, the comonomer partial pressure, and the production rate. The manipulated variables are selected as the catalyst feed rate, hydrogen feed rate, comonomer feed rate and the monomer feed rate. Process constraints are considered as described in the literature¹⁵⁾. The control interval is 1 min.

In order to provide off-set free estimation of the controlled variables, a simple multi-loop state estimator is designed. For example, in estimating the hydrogen partial pressure, an input disturbance ξ_h is assumed, and ξ_h

is updated by the hydrogen partial pressure measurement P_h and its estimate \hat{P}_h using the following equation:

$$\xi_h(t) = K_{c,h}(P_h - \hat{P}_h) + K_{I,h} \int_0^t (P_h - \hat{P}_h) d\tau, \quad (25)$$

where $K_{c,h}$, $K_{I,h}$ are tuning parameters.

Fig. 6 shows the closed-loop responses of the NMPC during a grade changeover, together with those of the LMPC under the same operating condition. In the figure, P_m , P_h/P_m , P_{ppp}/P_m denote the monomer partial pressure, the hydrogen/monomer partial pressure ratio and the comonomer/monomer partial pressure ratio respectively. Grade transition operations are realized by simply giving step changes to the setpoints of the controlled variable.

The NMPC improved the closed-loop performance, especially the monomer and hydrogen partial pressures responses. A long-term comparison of the NMPC and LMPC performances also confirmed the superiority of the developed NMPC to the conventional LMPC; the NMPC reduced the operator interventions by nearly two thirds and the service factors (the percentage of the time duration of the controller turned on) was increased by nearly 20%.

5. Conclusions

Nonlinear model predictive control based on successive linearization has been proposed. Through simulation studies on nonlinear chemical reactors which exhibit steady state input or output multiplicities, capability of the proposed controller has been demonstrated.

The developed control algorithm has been successfully applied to a grade transition operation in an industrial HDPE polymerization reactor.

Acknowledgment

The authors gratefully acknowledge Prof. Masahiro Ohshima of Kyoto University for his suggestion and guidance during the project for implementing NMPC on HDPE reactor.

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Hiroya SEKI (Member)



Hiroya Seki was born in July, 1963. He received M.E. degrees in mechanical engineering from Tokyo University in 1988, and Ph.D in chemical engineering from Kyoto University in 2002. He joined Mitsubishi Chemical Corporation in 1988 and was engaged in development of advanced control systems. Since 2005, he has been an Associate Professor at the Process Systems Engineering Division of Chemical Resources Laboratory, Tokyo Institute of Technology.

Satoshi Ooyama (Member)



Satoshi Ooyama was born in March, 1970. He received B.E degree in applied mathematics from Tokyo University. He joined Mitsubishi Chemical Corporation in 1993. Since then, he has been responsible to develop and implement advanced process control systems.

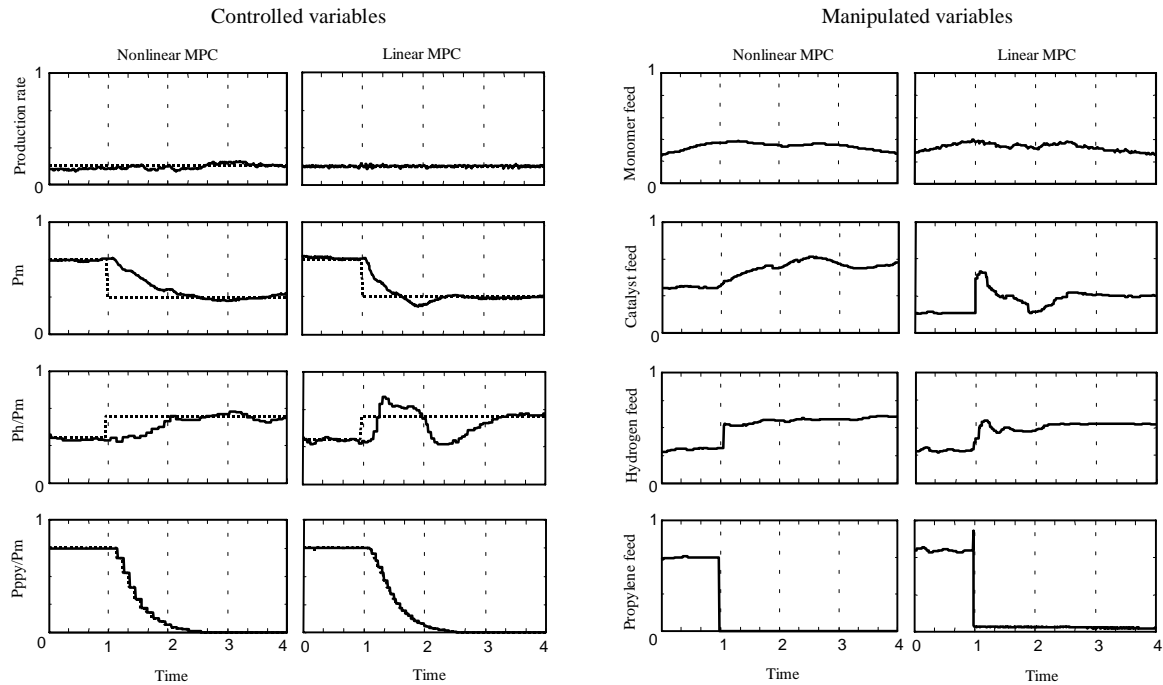


Fig. 6 Comparison of NMPC and LMPC responses in a grade changeover operation.

Morimasa OGAWA (Member)



Morimasa Ogawa was born in Kagawa, Japan, in 1948. He received Ph.D in chemical engineering from Kyoto University in 2001. He joined Mitsubishi Chemical Corporation in 1966 and was responsible to develop and implement advanced process control systems. Currently, he is a fellow of process control at Advanced Automation Company, Yamatake Corporation.