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Model predictive control of nonlinear processes

Ch. Venkateswarlu
Indian Institute of Chemical Technology

1. Historical background

Process control has become an integral part of process plants. An automatic controller must be able to facilitate the plant operation over a wide range of operating conditions. The proportional-integral (PI) or proportional-integral-derivative (PID) controllers are commonly used in many industrial control systems. These controllers are tuned with different tuning techniques to deliver satisfactory plant performance.

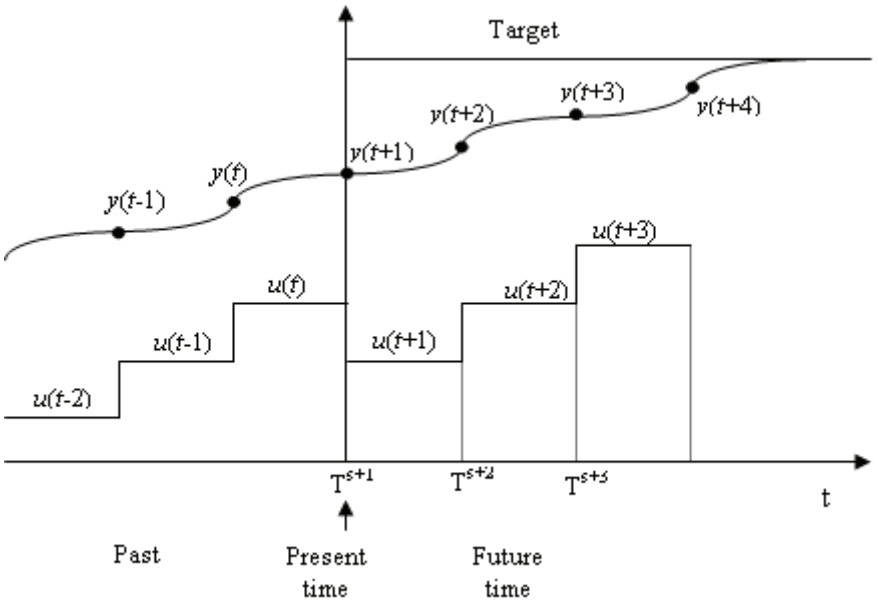

Fig. 1. MPC multi-step prediction scheme.

However, specific control problems associated with the plant operations severely limit the performance of conventional controllers. The increasing complexity of plant operations

together with tougher environmental regulations, rigorous safety codes and rapidly changing economic situations demand the need for more sophisticated process controllers.
Model predictive control (MPC) is an important branch of automatic control theory. MPC refers to a class of control algorithms in which a process model is used to predict and optimize the process performance. MPC has been widely applied in industry (Qin and Badgwell, 1997). The idea of MPC is to calculate a control function for the future time in order to force the controlled system response to reach the reference value. Therefore, the future reference values are to be known and the system behavior must be predictable by an appropriate model. The controller determines a manipulated variable profile that optimizes some open-loop performance objective over a finite horizon extending from the current time into the future. This manipulated variable profile is implemented until a plant measurement becomes available. Feedback is incorporated by using the measurement to update the optimization problem for the next time step. Figure 1 explains the basic idea of MPC showing how the past input-output information is used to predict the future process behavior at the current time and how this information is extended to future to track the desired setpoint trajectory. The notation y, u and T_s refer process output, control action and sample time, respectively.

2. Model predictive control scheme

Model predictive control (MPC) refers to a wide class of control algorithms that use an explicit process model to predict the behavior of a plant. The most significant feature that distinguishes MPC from other controllers is its long range prediction concept. This concept enables MPC to perform current computations to account the future dynamics, thus facilitating it to overcome the limitations of process dead time, non-minimum phase behavior and slow dynamics. In addition, MPC exhibits superior performance by systematically handling constraints violation.

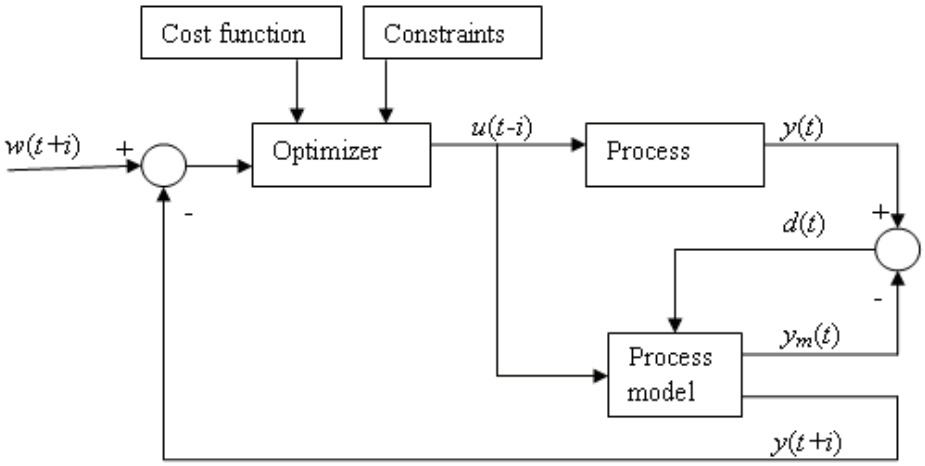

Fig. 2. MPC block diagram.

The fundamental framework of MPC algorithms is common for any kind of MPC schemes. The main differences in many MPC algorithms are the types models used to represent the plant dynamics and the cost function to be minimized. The multi-step model predictive control scheme shown in Figure 1 can be realized from the block diagram represented in Figure 2.

The basic elements in the block diagram are defined as follows. An appropriate model is used to predict the process outputs, $y(t+i), i=1,....,N$ over a future time interval known as prediction horizon, N. A sequence of control actions, $\Delta u(t+j)$, j=1,…., m over the control horizon m are calculated by minimizing some specified objective which is a function of predicted outputs, $y(t+i)$, set-point values, $w(t+i)$ and control actions, $\Delta u(t)$. The first control move, $u(t)$ of the sequence is implemented and the calculations are repeated for the subsequent sampling instants. In order to account the plant-model mismatch, a prediction error, $d(t)$, that is calculated based on plant measurement, $y(t)$ and model prediction, $y_m(t)$ is used to update the future predictions.

In MPC, the control law generates a control sequence, which forces the future system response to be equal to the reference values. The system response is based on future control actions, model parameters and the actual system states. Many methods for updating the optimization problem are possible, such as estimating model parameters and/or states, inferring about disturbances etc. MPC design considers different types of process models. These include first principle models, auto regressive moving average models, polynomial models, neural network models, fuzzy models etc. The attraction for MPC is due to its capability of handling various constraints directly in the formulation through on-line optimization. A variety of model predictive control techniques have been reported for controlling the processes of various complexities.

This chapter presents different linear and nonlinear model predictive controllers with case studies illustrating their application to real processes.

3. Linear model predictive control

Linear MPC (LMPC) algorithms employ linear or linearized models to obtain the predictive response of the controlled process. These algorithms include the Model Algorithmic Control (MAC) (Richalet et al., 1978), the Dynamic Matrix Control (DMC) (Cutler and Ramaker, 1980) and the Generalized Predictive Control (GPC) (Clarke et al., 1987). These algorithms are all similar in the sense that they rely on process models to predict the behavior of the process over some future time interval, and the control calculations are based on these model predictions. The models used for these predictions have usually been derived from linear approximations of the process or experimentally obtained step response data. A survey of theory and applications of such algorithms have been reported by Garcia et al. (1989).

3.1 LMPC design

A classical autoregressive moving average (ARX) model structure that relates the plant output with the present and past plant input-output can be used to formulate a predictive model. The model parameters can be determined a priori by using the known input-output data to form a fixed predictive model or these parameters are updated at each sampling

time by an adaptive mechanism. The one step ahead predictive model can be recursively extended to obtain future predictions for the plant output. The minimization of a cost function based on future plant predictions and desired plant outputs generates an optimal control input sequence to act on the plant. The strategy is described as follows.

Predictive model

The relation between the past input-output data and the predicted output can be expressed by an ARX model of the form

$$y(t+1) = a_1 y(t) + \ldots + a_{ny} y(t\text{-}ny+1) + b_1 u(t) + \ldots\ldots + b_{nu} u(t\text{-}nu+1) \tag{1}$$

where $y(t)$ and $u(t)$ are the process and controller outputs at time t, $y(t+1)$ is the one-step ahead model prediction at time t, a's and b's represent the model coefficients and the nu and ny are input and output orders of the system.

Model identification

The model output prediction can be expressed as

$$y_m(t+1) = \phi\, x_m(t) \tag{2}$$

where

$$\phi = [\alpha_1 \ldots \alpha_{ny}\ \beta_1 \ldots \beta_{nu}] \tag{3}$$

and

$$x_m(t) = [y(t) \ldots y(t\text{-}ny+1)\ \ u(t) \ldots u(t\text{-}nu+1)]^T \tag{4}$$

with α and β as identified model parameters.

One of the most widely used estimators for model parameters and covariance is the popular recursive least squares (RLS) algorithm (Goodwin and Sin, 1984). The RLS algorithm provides the updated parameters of the ARX model in the operating space at each sampling instant or these parameters can be determined a priori using the known data of inputs and outputs for different operating conditions. The RLS algorithm is expressed as

$$\begin{aligned} \phi(t+1) &= \phi(t) + K(t)\,[y(t+1) - y_m(t+1)] \\ K(t) &= P(t)\, x_m(t+1) \,/\, [1 + x_m(t+1)^T P(t)\, x_m(t+1)] \\ P(t+1) &= 1/\lambda\, [P(t) - \{(P(t)\, x_m(t+1)\, x_m(t+1)^T P(t)) \,/\, (1 + x_m(t+1)^T P(t)\, x_m(t+1))\}] \end{aligned} \tag{5}$$

where $\phi(t)$ represents the estimated parameter vector, λ is the forgetting factor, $K(t)$ is the gain matrix and $P(t)$ is the covariance matrix.

Controller formulation

The N time steps ahead output prediction over a prediction horizon is given by

$$y_p(t+N) = \alpha_1\ y(t+N\text{-}1)+\ldots+\alpha_{ny} y(t\text{-}ny+N)+\beta_1 u(t+N\text{-}1)+\ldots+\beta_{nu} u(t\text{-}nu+N)+err(t) \tag{6}$$

where $y_p(t+N)$ represent the model predictions for N steps and $err(t)$ is an estimate of the modeling error which is assumed as constant for the entire prediction horizon. If the control horizon is m, then the controller output, u after m time steps can be assumed to be constant.

An internal model is used to eliminate the discrepancy between model and process outputs, *error*(*t*), at each sampling instant

$$error(t) = y(t) - y_m(t) \tag{7}$$

where $y_m(t)$ is the one-step ahead model prediction at time (t-1). The estimate of the error is then filtered to produce *err*(*t*) which minimizes the instability introduced by the modeling error feedback. The filter error is given by

$$err(t) = (1\text{-}K_f)\, err(t\text{-}1) + K_f\, error(t) \tag{8}$$

where K_f is the feedback filter gain which has to be tuned heuristically.
Back substitutions transform the prediction model equations into the following form

$$\begin{aligned} & y_p(t+N) = f_{N,1}y(t) + ... + \\ & f_{N,ny}y(t-ny+1) + f_{N,ny+1}u(t-1) + \\ & .....+ f_{N,ny+nu-1}u(t-nu+1) + \\ & g_{N,1}u(t) + ... + g_{N,m}u(t+m-1) \\ & + e_N err(t) \end{aligned} \tag{9}$$

The elements *f*, *g* and *e* are recursively calculated using the parameters α and β of Eq. (3). The above equations can be written in a condensed form as

$$Y(t) = F\,X(t) + G\,U(t) + E\,err(t) \tag{10}$$

where

$$Y(t) = [y_p(t\text{+}1) \ldots y_p(t\text{+}N)]^T \tag{11}$$

$$X(t) = [y(t)\ \ y(t\text{-}1) \ldots y(t\text{-}ny\text{+}1)\ \ u(t\text{-}1) \ldots u(t\text{-}nu\text{+}1)]^T \tag{12}$$

$$U(t) = [u(t) \ldots u(t\text{+}m\text{-}1)]^T \tag{13}$$

$$F = \begin{bmatrix} f_{11}\ f_{12}\ \cdots\cdots f_{1(ny+nu-1)} \\ f_{11}\ f_{12}\ \cdots\cdots f_{2(ny+nu-1)} \\ \vdots \\ \vdots \\ f_{N1}\ f_{N12}\ \cdots\cdots f_{N(ny+nu-1)} \end{bmatrix}$$

$$G = \begin{bmatrix} g_{11} & 0 & 0 & \ldots & 0 \\ g_{21} & g_{21} & 0 & \ldots & 0 \\ . & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \\ g_{m1} & g_{m2} & g_{m3} & \cdots & g_{mm} \\ . & . & . & \ldots & . \\ . & . & . & \ldots & . \\ . & . & . & \ldots & . \\ g_{N1} & g_{N2} & g_{N3} & \cdots & g_{Nm} \end{bmatrix}$$

$$E = [e_1 \ldots e_N]^T$$

In the above, $Y(t)$ represents the model predictions over the prediction horizon, $X(t)$ is a vector of past plant and controller outputs and $U(t)$ is a vector of future controller outputs. If the coefficients of F, G and E are determined then the transformation can be completed. The number of columns in F is determined by the ARX model structure used to represent the system, where as the number of columns in G is determined by the length of the control horizon. The number of rows is fixed by the length of the prediction horizon.

Consider a cost function of the form

$$J = \sum_{i=1}^{N} \left[y_p(t+i) - w(t+i) \right]^2 + \sum_{i=1}^{m} \gamma \left[u(t+i-1 \right]^2$$

$$= \sum_{i=1}^{N} \left[Y(t) - W(t) \right]^T \left[Y(t) - W(t) \right] + \sum_{i=1}^{m} \gamma U(t)^T U(t) \tag{14}$$

where $W(t)$ is a setpoint vector over the prediction horizon

$$W(t) = [\, w(t+1) \ldots . w(t+N)]^T \tag{15}$$

The minimization of the cost function, J gives optimal controller output sequence

$$U(t) = [G^T G + \gamma I\,]^{-1} G^T [W(t) - FX(t) - Eerr(t)] \tag{16}$$

The vector $U(t)$ generates control sequence over the entire control horizon. But, the first component of $U(t)$ is actually implemented and the whole procedure is repeated again at the next sampling instant using latest measured information.
Linear model predictive control involving input-output models in classical, adaptive or fuzzy forms is proved useful for controlling processes that exhibit even some degree of nonlinear behavior (Eaton and Rawlings, 1992; Venkateswarlu and Gangiah, 1997 ; Venkateswarlu and Naidu, 2001).

3.2 Case study: linear model predictive control of a reactive distillation column

In this study, a multistep linear model predictive control (LMPC) strategy based on autoregressive moving average (ARX) model structure is presented for the control of a reactive distillation column. Although MPC has been proved useful for a variety of chemical and biochemical processes (Garcia et al., 1989 ; Eaton and Rawlings, 1992), its application to a complex dynamic system like reactive distillation is more interesting.

The process and the model

Ethyl acetate is produced through an esterfication reaction between acetic acid and ethyl alcohol

$$CH_3COOH + C_2H_5OH \xleftrightarrow{H+} H_2O + CH_3COOC_2H_5 \tag{17}$$

The achievable conversion in this reversible reaction is limited by the equilibrium conversion. This quaternary system is highly non-ideal and forms binary and ternary

azeotropes, which introduce complexity to the separation by conventional distillation. Reactive distillation can provide a means of breaking the azeotropes by altering or eliminating the conditions for azeotrope formation. Thus reactive distillation becomes attractive alternative for the production of ethyl acetate.
The rate equation of this reversible reaction in the presence of a homogeneous acid catalyst is given by (Alejski and Duprat, 1996)

$$\begin{aligned} r_1 &= k_1 C_1 C_2 - \frac{k_1}{K_c} C_3 C_4 \\ k_1 &= (4.195 C_k + 0.08815) \exp(-6500.1/T) \\ K_c &= 7.558 - 0.012T \end{aligned} \tag{18}$$

Vora and Daoutidis (2001) have presented a two feed column configuration for ethyl acetate reactive distillation and found that by feeding the two reactants, ethanol and acetic acid, on different trays counter currently allows to enhance the forward reaction on trays and results in higher conversion and purity over the conventional column configuration of feeding the reactants on a single tray. All plates in the column are considered to be reactive. The column consists of 13 stages including the reboiler and the condenser. The less volatile acetic acid enters the 3 rd tray and the more volatile ethanol enters the 10 th tray. The steady state operating conditions of the column are shown in Table 1.

Acetic acid feed flow rate, F_{Ac}	6.9 mol/s
Ethanol flow rate, F_{Eth}	6.865 mol/s
Reflux flow rate, L_o	13.51 mol/s
Distillate flow rate, D	6.68 mol/s
Bottoms flow rate, B	7.085 mol/s
Reboiler heat duty, Q_r	5.88 x 10^5 J/mol
Boiling points, ^oK	391.05, 351.45, 373.15, 350.25
(Acetic acid, ethanol, water, ethyl acetate)	
Distillate composition	0.0842, 0.1349, 0.0982, 0.6827
(Acetic acid, ethanol, water, ethyl acetate)	
Bottoms composition	0.1650, 0.1575, 0.5470, 0.1306
(Acetic acid, ethanol, water, ethyl acetate)	

Table 1. Design conditions for ethyl acetate reactive distillation column

The dynamic model representing the process operation involves mass and component balance equations with reaction terms, along with energy equations supported by vapor-liquid equilibrium and physical properties (Alejski & Duprat, 1996). The assumptions made in the formulation of the model include adiabatic column operation, negligible heat of reaction, negligible vapor holdup, liquid phase reaction, physical equilibrium in streams leaving each stage, negligible down comer dynamics and negligible weeping of liquid through the openings on the tray surface. The equations representing the process are given as follows.

Total mass balance

Total condenser:

$$\frac{dM_1}{dt} = V_2 - (L_1 + D) + \Delta R_1 \tag{19}$$

Plate j:

$$\frac{dM_j}{dt} = FV_j + V_{j+1} + FL_j + L_{j-1} - V_j - L_j + \Delta R_j \tag{20}$$

Reboiler :

$$\frac{dM_n}{dt} = L_{n-1} - V_n - L_n + \Delta R_n \tag{21}$$

Component mass balance

Total condenser :

$$\frac{d(M_1 x_{i,1})}{dt} = V_2 y_{i,2} - (L_1 + D)x_{i,1} + R_{i,1} \tag{22}$$

Plate j:

$$\frac{d(M_j x_{i,j})}{dt} = FV_j yf_{i,j} + V_{j+1} y_{i,j+1} + FL_j xf_{i,j} + L_{j-1} x_{i,j-1} - V_j y_{i,j} - L_j x_{i,j} + R_{i,j} \tag{23}$$

Reboiler:

$$\frac{d(M_n x_{i,n})}{dt} = L_{n-1} x_{i,n-1} - V_n y_{i,n} - L_n x_{i,n} + R_{i,n} \tag{24}$$

Total energy balance

Total condenser :

$$\frac{dE_1}{dt} = V_2 H_2 - (L_1 + D)h_1 + Q_1 \tag{25}$$

Plate j:

$$\frac{dE_j}{dt} = FV_j Hf_j + V_{j+1} H_{j+1} + FL_j hf_j + L_{j-1} h_{j-1} - V_j H_j - L_j h_j + Q_j \tag{26}$$

Reboiler:

$$\frac{dE_n}{dt} = L_{n-1} h_{n-1} - V_n H_n - L_n h_n + Q_n \tag{27}$$

Level of liquid on the tray

$$L^{liq} = \frac{M_n MW_{av}}{A_{tray} \rho_{av}} \tag{28}$$

Flow of liquid over the weir

$$\text{If } (L^{liq} < h_{weir}) \text{ then } L_n = 0 \tag{29}$$

else

$$L_n = 1.84 \frac{L_{weir}\rho_{av}}{MW_{av}} (L^{liq} - h_{weir})^{3/2} \tag{30}$$

Mole fraction normalization

$$\sum_{i=1}^{NC} x_i = \sum_{i=1}^{NC} y_i = 1 \tag{31}$$

VLE calculations

For the column operation under moderate pressures, the VLE equation assumes the ideal gas model for the vapor phase, thus making the vapor phase activity coefficient equal to unity. The VLE relation is given by

$$y_i P = x_i \gamma_i P_i^{sat} \qquad (i = 1,2,\ldots,NC) \tag{32}$$

The liquid phase activity coefficients are calculated using UNIFAC method (Smith et al., 1996).

Enthalpies Calculation
The relations for the liquid enthalpy h, the vapor enthalpy H and the liquid density ρ are:

$$\begin{aligned} h &= h(P, T, x) \\ H &= H(P, T, y) \\ \rho^{liq} &= \rho^{liq}(P, T, x) \end{aligned} \tag{33}$$

Control scheme

The design and implementation of the control strategy is studied for the single input-single output (SISO) control of the ethyl acetate reactive distillation column with its double feed configuration. The objective is to control the desired product purity in the distillate stream inspite disturbances in column operation. This becomes the main control loop. Since reboiler and condenser holdups act as pure integrators, they also need to be controlled. These become the auxiliary control loops. Reflux flow rate is used as a manipulated variable to control the purity of the ethyl acetate. Distillate flow rate is used as a manipulated variable to control the condenser holdup, while bottom flow rate is used to control the reboiler holdup. In this work, it is proposed to apply a multistep model predictive controller for the main loop and conventional PI controllers for the auxiliary control loops. This control scheme is shown in the Figure 3.

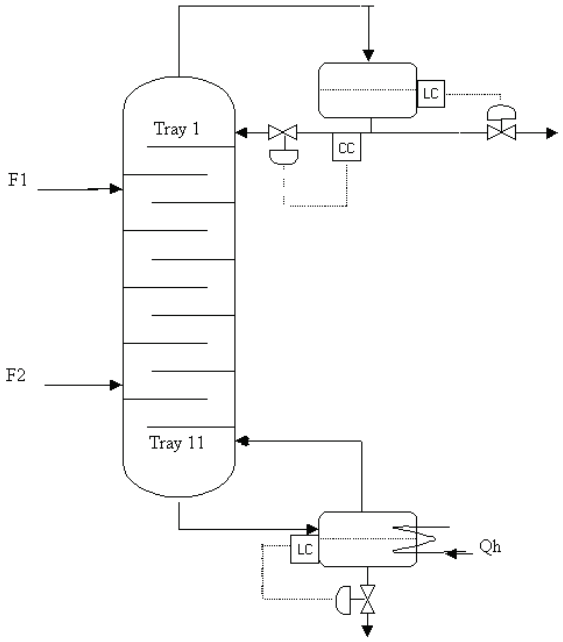

Fig. 3. Control structure of two feed ethyl acetate reactive distillation column.

Analysis of Results

The performance of the multistep linear model predictive controller (LMPC) is evaluated through simulation. The product composition measurements are obtained by solving the model equations using Euler's integration with sampling time of 0.01 s. The input and output orders of the predictive model are considered as n_u = 2 and n_y = 2. The diagonal elements of the initial covariance matrix, $P(0)$ in the RLS algorithm are selected as 10.0, 1.0, 0.01, 0.01, respectively. The forgetting factor, λ used in recursive least squares is chosen as 5.0. The feedback controller gain K_f is assigned as 0.65. The tuning parameter γ in the control law is set as 0.115 x 10^{-6}. The PI controller parameters of ethyl acetate composition are evaluated by using the continuous cycling method of Ziegler and Nichols. The tuned controller settings are k_c = 11.15 and τ_I = 1.61 x 10^4 s. The PI controller parameters used for reflux drum and reboiler holdups are k_c = - 0.001 and τ_I = 5.5 h, and k_c = - 0.001 and τ_I = 5.5 h, respectively (Vora and Daoutidis, 2001).

The LMPC is implemented by adaptively updating the prediction model using recursive least squares. On evaluating the effect of different prediction and control horizons, it is observed that the LMPC with a prediction horizon of around 5 and a control horizon of 2 has shown reasonably better control performance. The LMPC is also referred here as MPC. Figure 4 shows the results of MPC and PI controller when they are applied for tracking series of step changes in ethyl acetate composition. The regulatory control performance of MPC and PI controller for 20% decrease in feed rate of acetic acid is shown in Figure 5. The results thus show the effectiveness of the multistep linear model predictive control strategy for the control of highly nonlinear reactive distillation column.

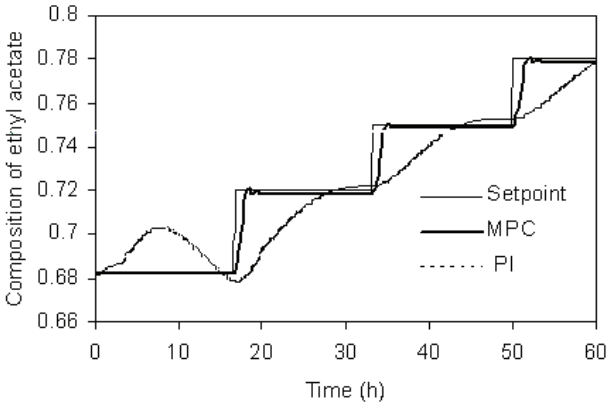

Fig. 4. Performance of MPC and PI controller for tracking series of step changes in distillate composition.

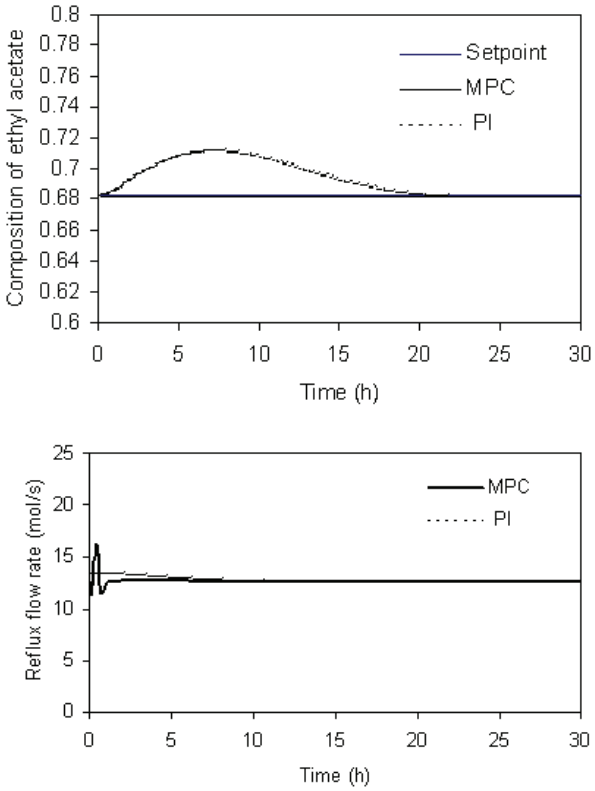

Fig.5. Output and input profiles for MPC and PI controller for 20% decrease in the feed rate of acetic acid.

4. Generalized predictive control

The generalized predictive control (GPC) is a general purpose multi-step predictive control algorithm (Clarke et al., 1987) for stable control of processes with variable parameters, variable dead time and a model order which changes instantaneously. GPC adopts an integrator as a natural consequence of its assumption about the basic plant model. Although GPC is capable of controlling such systems, the control performance of GPC needs to be ascertained if the process constraints are to be encountered in nonlinear processes. Camacho (1993) proposed a constrained generalized predictive controller (CGPC) for linear systems with constrained input and output signals. By this strategy, the optimum values of the future control signals are obtained by transforming the quadratic optimization problem into a linear complementarity problem. Camacho demonstrated the results of the CGPC strategy by carrying out a simulation study on a linear system with pure delay. Clarke et al. (1987) have applied the GPC to open-loop stable unconstrained linear systems. Camacho applied the CGPC to constrained open-loop stable linear system. However, most of the real processes are nonlinear and some processes change behavior over a period of time. Exploring the application of GPC to nonlinear process control will be more interesting.
In this study, a constrained generalized predictive control (CGPC) strategy is presented and applied for the control of highly nonlinear and open-loop unstable processes with multiple steady states. Model parameters are updated at each sampling time by an adaptive mechanism.

4.1 GPC design

A nonlinear plant generally admits a local-linearized model when considering regulation about a particular operating point. A single-input single-output (SISO) plant on linearization can be described by a Controlled Autoregressive Integrated Moving Average (CARIMA) model of the form

$$A(q^{-1})y(t) = B(q^{-1})q^{-d}\,u(t) + C\,(q^{-1})e(t\,)/\Delta \tag{34}$$

where A, B and C are polynomials in the backward shift operator q^{-1}. The $y(t)$ is the measured plant output, $u(t)$ is the controller output, $e(t)$ is the zero mean random Gaussian noise, d is the delay time of the system and Δ is the differencing operator $1\text{-}q^{-1}$.
The control law of GPC is based on the minimization of a multi-step quadratic cost function defined in terms of the sum of squares of the errors between predicted and desired output trajectories with an additional term weighted by projected control increments as given by

$$J(N_1, N_2, N_3) = E\left\{ \sum_{j=N_1}^{N_2} \{[y(t+j|t) - w(t+j)]^2 \; + \sum_{j=1}^{N_3} \lambda[\Delta u(t+j-1)]^2 \right\} \tag{35}$$

where $E\{.\}$ is the expectation operator, $y(t + j \mid t\,)$ is a sequence of predicted outputs, $w(t + j)$ is a sequence of future setpoints, $\Delta u(t + j\text{ -}1)$ is a sequence of predicted control increments and λ is the control weighting factor. The N_1 , N_2 and N_3 are the minimum costing horizon, the maximum costing horizon and the control horizon, respectively. The values of N_1 , N_2 and N_3 of Eq. (35) can be defined by $N_1 = d + 1$, $N_2 = d + N$, and $N_3 = N$, respectively.

Predicting the output response over a finite horizon beyond the dead-time of the process enables the controller to compensate for constant or variable time delays. The recursion of the Diophantine equation is a computationally efficient approach for modifying the predicted output trajectory. An optimum *j*-step a head prediction output is given by

$$y(t+j \mid t) = G_j(q^{-1})\,\Delta u(t+j-d-1) + F_j(q^{-1})y(t) \tag{36}$$

where $G_j(q^{-1}) = E_j(q^{-1})B(q^{-1})$, and E_j and F_j are polynomials obtained recursively solving the Diophantine equation,

$$1 = E_j(q^{-1})A\Delta + q^{-j}F_j(q^{-1}) \tag{37}$$

The *j*-step ahead optimal predictions of y for $j = 1, \ldots, N_2$ can be written in condensed form

$$Y = Gu + f \tag{38}$$

where f contains predictions based on present and past outputs up to time t and past inputs and referred to free response of the system, i.e., $f = [f_1, f_2, \ldots, f_N]$. The vector u corresponds to the present and future increments of the control signal, *i.e.*, $u = [\Delta u(t), \Delta u(t+1), \ldots, \Delta u(t+N-1)]^T$. Eq. (35) can be written as

$$J = \left(Gu + f - w\right)^T \left(Gu + f - w\right) + \lambda\, u^T u \tag{39}$$

The minimization of J gives unconstrained solution to the projected control vector

$$u = (G^T G + \lambda I)^{-1} G^T (w - f) \tag{40}$$

The first component of the vector u is considered as the current control increment $\Delta u(t)$, which is applied to the process and the calculations are repeated at the next sampling instant. The schematic of GPC control law is shown in Figure 6, where K is the first row of the matrix $(G^T G + \lambda I)^{-1} G^T$.

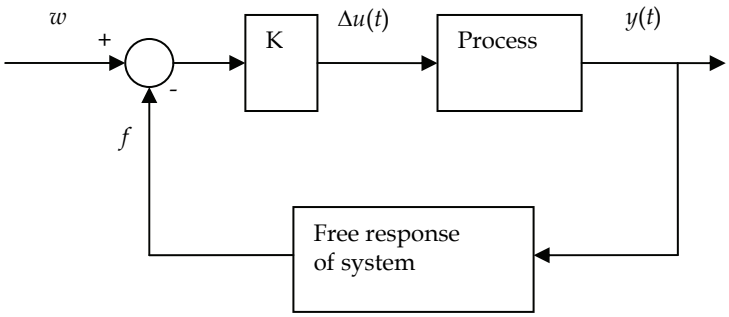

Fig. 6. The GPC control law

4.2 Constrained GPC design

In practice, all processes are subject to constraints. Control valves are limited by fully closed and fully open positions and maximum slew rates. Constructive and safety reasons as well as sensor ranges cause limits in process variables. Moreover, the operating points of plants are determined in order to satisfy economic goals and usually lie at the intersection of certain constraints. Thus, the constraints acting on a process can be manipulated variable limits (u_{min}, u_{max}), slew rate limits of the actuator (du_{min}, du_{max}), and limits on the output signal (y_{min}, y_{max}) as given by

$$\begin{aligned} u_{\min} &\le u(t) \le u_{\max} \\ du_{\min} &\le u(t) - u(t-1) \le du_{\max} \\ y_{\min} &\le y(t) \le y_{\max} \end{aligned} \tag{41}$$

These constraints can be expressed as

$$\begin{aligned} lu_{\min} &\le Tu + u(t-1)l \le lu_{\max} \\ ldu_{\min} &\le u \le ldu_{\max} \\ ly_{\min} &\le Gu + f \le ly_{\max} \end{aligned} \tag{42}$$

where l is an N vector containing ones, and T is an N x N lower triangular matrix containing ones. By defining a new vector $x = u - ldu_{min}$, the constrained equations can be transformed as

$$\begin{aligned} x &\ge 0 \\ Rx &\le c \end{aligned} \tag{43}$$

with

$$R = \begin{bmatrix} I_{NxN} \\ T \\ -T \\ G \\ -G \end{bmatrix} \quad ; \qquad c = \begin{bmatrix} l(du_{\max} - du_{\min}) \\ lu_{\max} - Tldu_{\min} - u(t-1)l \\ -lu_{\min} + Tldu_{\min} + u(t-1)l \\ ly_{\max} - f - Gldu_{\min} \\ -ly_{\min} + f + Gldu_{\min} \end{bmatrix} \tag{44}$$

Eq. (39) can be expressed as

$$J = \frac{1}{2} u^T Hu + bu + f_o \tag{45}$$

where

$$H = 2(G^T G + \lambda I)$$
$$b = G^T (f - w) + (f - w)^T G$$
$$f_o = (f - w)^T (f - w)$$

The minimization of J with no constraints on the control signal gives

$$u = -H^{-1} b \tag{46}$$

Eq. (45) in terms of the newly defined vector x becomes

$$J = \frac{1}{2} x^T H x + a x + f_1 \tag{47}$$

where

$$a = b + u_{\min} l^T H$$
$$f_1 = f_o + \frac{1}{2} d u_{\min}^2 l^T H l + b l d u_{\min}$$

The solution of the problem can be obtained by minimization of Eq. (47) subject to the constraints of Eq. (43). By using the Lagrangian multiplier vectors v_1 and v for the constraints, $x \geq 0$ and $Rx \leq c$, respectively, and introducing the slack variable vector v_2, the Kuhn-Tucker conditions can be expressed as

$$\begin{aligned} & Rx + v_2 = c \\ & -Hx - R^T v + v_1 = a \\ & x^T v_1 = 0 \\ & v^T v_2 = 0 \\ & x, v, v_1, v_2 \geq 0 \end{aligned} \tag{48}$$

Camacho (1993) has proposed the solution of this problem with the help of Lemke's algorithm (Bazaraa and Shetty, 1979) by expressing the Kuhn-Tucker conditions as a linear complementarity problem starting with the following tableau

	v_2	x	v	v_1	z_0	
v_2	I_{mxn}	O_{mxN}	$-RH^{-1}R^T$	RH^{-1}	-1	$v_{2\min}$
x	O_{Nxm}	I_{NxN}	$H^{-1}R^T$	$-H^{-1}$	-1	$x_{\min}$

(49)

Here, z_0 is the artificial variable which will be driven to zero iteratively.

In this study, the above stated constrained generalized predictive linear control of Camacho (1993) is extended to open-loop unstable constrained control of nonlinear processes. In this

strategy, process nonlinearities are accounted through adaptation of model parameters while taking care of input and output constraints acting on the process. The following recursive least squares formula (Hsia, 1977) is used for on-line estimation of parameters and the covariance matrix after each new sample:

$$\begin{aligned}\theta(k+1) &= \theta(k) + \gamma(k+1)P(k)v(k+1)\left[y(k+1) - v^T(k+1)\theta(k)\right] \\ P(k+1) &= \frac{1}{\lambda}\left[P(k) - \gamma(k+1)P(k)v(k+1)v^T(k+1)P(k)\right] \\ \gamma(k+1) &= 1 \Big/ \left[1 + v^T(k+1)P(k)v(k+1)\right]\end{aligned} \tag{50}$$

where θ is the parameter vector, γ is the intermediate estimation variable, P is the covariance matrix, v is the vector of input-output variables, y is the output variable, and $0 < \lambda < 1$ is the forgetting factor. The initial covariance matrix and exponential forgetting factor are selected based on various trials so as to provide reasonable convergence in parameter estimates.

The CGPC strategy of nonlinear processes is described in the following steps:

1. Specify the controller design parameters N_1, N_2, N_3 and also the initial parameter estimates and covariance matrix for recursive identification of model parameters.
2. Update the model parameters using recursive least squares method.
3. Initialize the polynomials E_1 and F_1 of Diophantine identity, Eq. (37), using the estimated parameters. Further initialize G_1 as $E_1 B$.
4. Compute the polynomials E_j , F_j and G_j over the prediction horizon and control horizon using the recursion of Diophantine.
5. Compute matrices H, R, and G, and vectors f and c using the polynomials determined in step 4.
6. Compute the unconstrained solution $x_{min} = - H^{-1} a$.
7. Compute $v_{2min} = c - Rx_{min}$. If x_{min} and v_{2min} are nonnegative, then go to step 10.
8. Start Lemke's algorithm with x and v_2 in the basis with the tableau, Eq. (49).
9. If x_1 is not in the first column of the tableau, make it zero; otherwise, assign it the corresponding value.
10. Compute $u(t) = x_1 + du_{min} + u(t - 1)$.
11. Implement the control action, then shift to the next sampling instant and go to step 2.

4.3 Case study: constrained generalized predictive control (CGPC) of open-loop unstable CSTR

The design and implementation of the CGPC strategy is studied by applying it for the control of a nonlinear open-loop unstable chemical reactor (Venkateswarlu and Gangiah, 1997).

Reactor

A continuous stirred tank reactor (CSTR) in which a first order exothermic irreversible reaction occurs is considered as an example of an unstable nonlinear process. The dynamic equations describing the process can be written as

$$V\frac{dC_A}{dt'} = F(C_{Af} - C_A) - Vk_0 \exp\left[-E / R_g T_r\right] C_A \tag{51}$$

$$V\rho C_p \frac{dT_r}{dt'} = \rho C_p F(T_f - T_r) + V(-\Delta H)k_0 \exp\left[-E / R_g T_r\right] C_A - UA_h(T_r - T_c) \tag{52}$$

where C_A and T_r are reactant concentration and temperature, respectively. The coolant temperature T_c is assumed to be the manipulated variable. Following the analysis of Uppal et al. (1974), the model is made dimensionless by introducing the parameters as

$$\phi = \frac{E}{R_g T_{fo}}, \quad B_h = \frac{(-\Delta H)C_{Afo}}{\rho C_p T_{fo}}, \quad D_a = \frac{k_o e^{-\phi} V}{F_o}, \quad \beta = \frac{UA_h}{F_o \rho C_p} \tag{53}$$

where F_o, C_{Afo} and T_{fo} are the nominal characteristic values of volumetric flow rate, feed composition and feed temperature, respectively. The corresponding dimensionless variables are defined by

$$t = \frac{t'F_o}{V}, \quad x_1 = \frac{C_{Afo} - C_A}{C_{Afo}}, \quad x_2 = \frac{T_r - T_{fo}}{T_{fo}}, \quad u = \frac{T_c - T_{co}}{T_{fo}}\phi \tag{54}$$

where T_{co} is some reference value for the coolant temperature.
The modeling equations can be written in dimensionless form (Calvet and Arkun, 1988; Hernandez and Arkun, 1992) as

$$\dot{x}_1 = -x_1 + Da(1 - x_1)\exp\left(\frac{x_2}{1 + x_2/\phi}\right)$$

$$\dot{x}_2 = -x_2 + B_h Da(1 - x_1)\exp\left(\frac{x_2}{1 + x_2/\phi}\right) + \beta(u - x_2) \tag{55}$$

$$y = x_1$$

where x_1 and x_2 are the dimensionless reactant concentration and temperature, respectively. The input u is the cooling jacket temperature, D_a is the Damkohler number, ϕ is the dimensionless activation energy, B_h is the heat of reaction and β is the heat transfer coefficient. If the physical parameters chosen are $D_a = 0.072$, $\phi = 20.0$, $B_h = 8.0$, and $\beta = 0.3$, then the system can exhibit up to three steady states, one of which is unstable as shown in Figure 7. Here the task is to control the reactor at and around the unstable operating point. The cooling water temperature is the input u, which is the manipulated variable to control the reactant concentration, x_1.

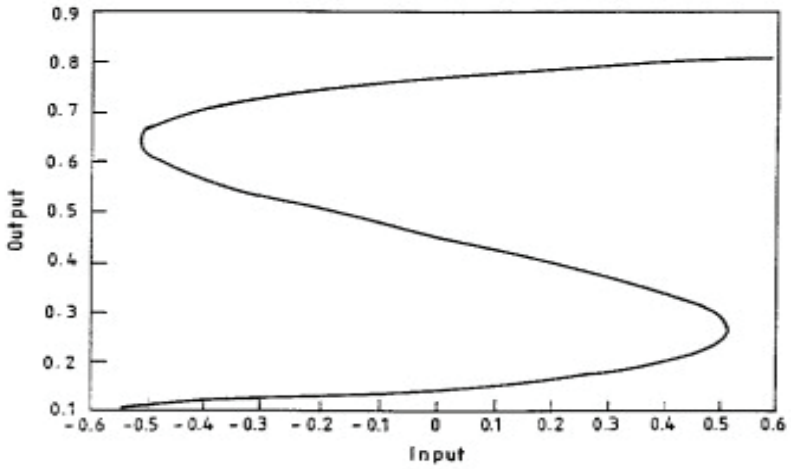

Fig. 7. Steady state output vs. steady state input for CSTR system.

Analysis of Results

Simulation studies are carried out in order to evaluate the performance of the Constrained Generalized Predictive Control (CGPC) strategy. The results of unconstrained Generalized Predictive Control (GPC) are also presented as a reference. The CGPC strategy considers an adaptation mechanism for model parameters.

N_a	2
N_b	2
N_1	2
N_2	7
N_3	6
λ	0.2
u_{min}	-1.0
u_{max}	1.0
du_{min}	-0.5
du_{max}	0.5
y_{min}	0.1
y_{max}	0.5
Forgetting factor	0.95
Initial covariance matrix	$1.0x10^9$
Sample time	0.5

Table 2. Constraints and parameters of CSTR system.

The controller and design parameters as well as the constraints employed for the CSTR system are given in Table 2. The same controller and design parameters are used for both the CGPC and GPC. Two set-point changes are introduced for the output concentration of the system and the corresponding results of CGPC and GPC are analyzed. A step change is

introduced in the output concentration of *CSTR* from a stable equilibrium point (x_1 = 0.2, x_2 = 1.33, u = 0.42) to an unstable operating point (x_1 = 0.5, x_2 = 3.303, u = - 0.2). The input and output responses of both CGPC and GPC are shown in Figure 8. Another step change is introduced for the set-point from a stable operating point (x_1 = 0.144, x_2 = 0.886, u = 0.0) to an unstable operating point (x_1 = 0.445, x_2 = 2.75, u = 0.0). The input and output responses of CGPC and GPC for this case are shown in Figure 9. The results show that for the specified controller and design parameters, CGPC provides better performance over GPC.

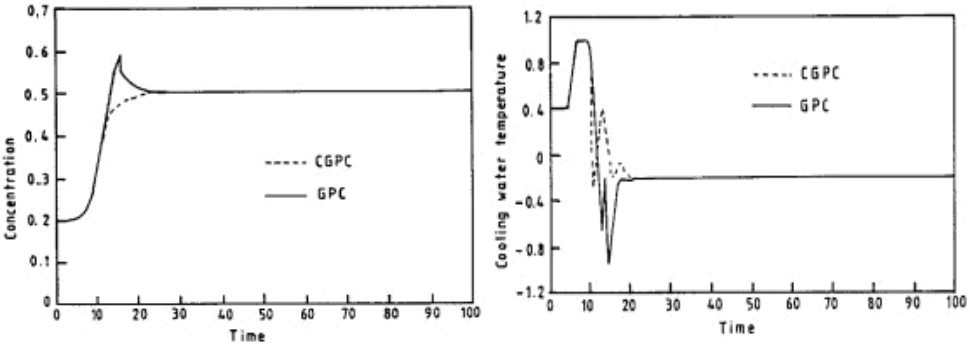

Fig. 8. Cooling water temperature and concentration plots of CSTR for a step change in concentration from 0.20 to 0.50.

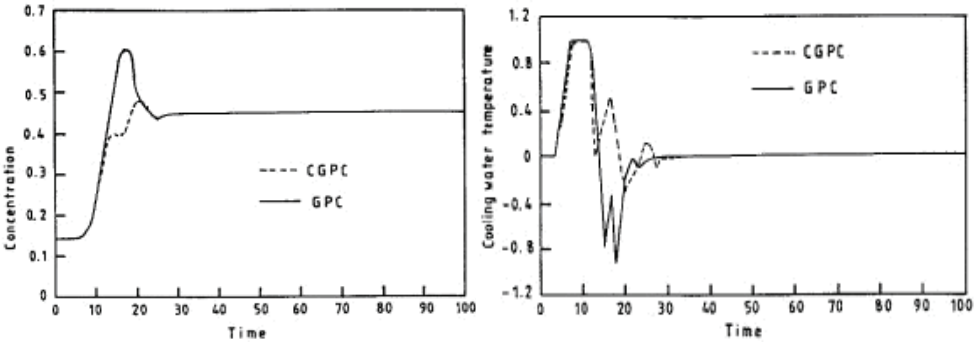

Fig. 9. Cooling water temperature and concentration plots of CSTR for a step change in concentration from 0.144 to 0.445.

The results illustrate the better performance of CGPC for SISO control of nonlinear systems that exhibit multiple steady states and unstable behavior.

5. Nonlinear model predictive control

Linear MPC employs linear or linearized models to obtain the predictive response of the controlled process. Linear MPC is proved useful for controlling processes that exhibit even some degree of nonlinear behavior (Eaton and Rawlings, 1992; Venkateswarlu and Gangiah, 1997). However, the greater the mismatch between the actual process and the representative

model, the degree of deterioration in the control performance increases. Thus the control of a highly nonlinear process by MPC requires a suitable model that represents the salient nonlinearities of the process. Basically, two different approaches are used to develop nonlinear dynamic models. These approaches are developing a first principle model using available process knowledge and developing an empirical model from input-output data. The first principle modeling approach results models in the form of coupled nonlinear ordinary differential equations and various model predictive controllers based on this approach have been reported for nonlinear processes (Wright and Edgar, 1994 ; Ricker and Lee, 1995). The first principle models will be larger in size for high dimensional systems thus limiting their usage for MPC design. On the other hand, the input-output modeling approach can be conveniently used to identify nonlinear empirical models from plant data, and there has been a growing interest in the development of different types of MPCs based on this approach (Hernandez and Arkun, 1994; Venkateswarlu and Venkat Rao, 2005). The other important aspect in model predictive control of highly nonlinear systems is the optimization algorithm. Efficient optimization algorithms exist for convex optimization problems. However, the optimization problem often becomes nonconvex in the presence of nonlinear characteristics/constraints and is usually more complex than convex optimization. Thus, the practical usefulness of nonlinear predictive control is hampered by the unavailability of suitable optimization tools (Camacho and Bordons, 1995). Sequential quadratic programming (SQP) is widely used classical optimization algorithm to solve nonlinear optimization problems. However, for the solution of large problems, it has been reported that gradient based methods like SQP requires more computational efforts (Ahn et al., 1999). More over, classical optimization methods are more sensitive to the initialization of the algorithm and usually leads to unacceptable solutions due to convergence to local optima. Consequently, efficient optimization techniques are being used to achieve the improved performance of NMPC.

This work presents a NMPC based on stochastic optimization technique. Stochastic approach based genetic algorithms (GA) and simulated annealing (SA) are potential optimization tools because of their ability to handle constrained, nonlinear and nonconvex optimization problems. These methods have the capacity to escape local optima and find solutions in the vicinity of the global optimum. They have the ability to use the values from the model in a black box optimization approach with out requiring the derivatives. Various studies have been reported to demonstrate the ability of these methods in providing efficient optimization solutions (Hanke and Li, 2000 ; Shopova and Vaklieva-Bancheva, 2006).

5.1 NMPC design

In NMPC design, the identified input-output nonlinear process model is explicitly used to predict the process output at future time instants over a specified prediction horizon. A sequence of future control actions over a specified control horizon is calculated using a stochastic optimizer which minimizes the objective function under given operating constraints. In this receding horizon approach, only the first control action in the sequence is implemented. The horizons are moved towards the future. The structure of the stochastic optimizer based NMPC is shown in Figure 10.

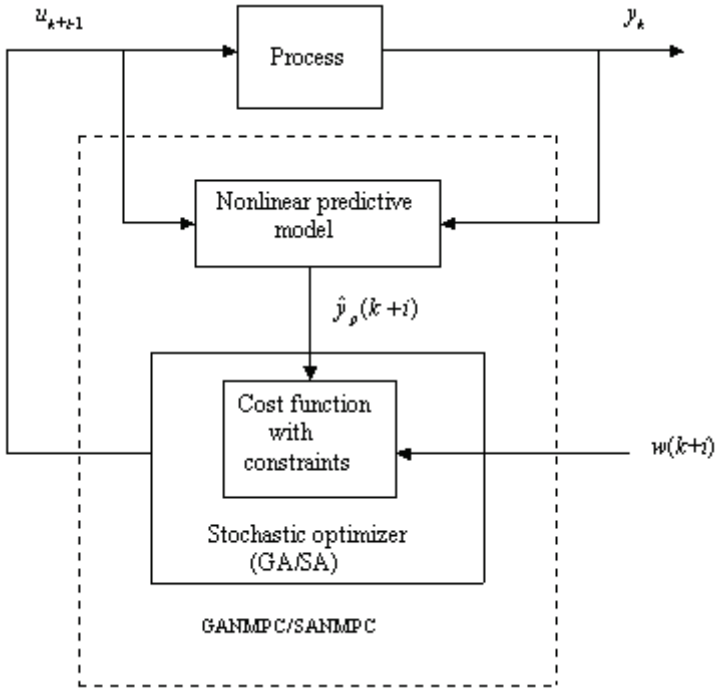

Fig.10. Structure of stochastic optimization based NMPC.

Simulated Annealing

Simulated annealing (SA) is analogous to the process of atomic rearrangement of a substance into a highly ordered crystalline structure by way of slowly cooling-annealing the substance through successive stages. This method is found to be a potential tool to solve a variety of optimization problems (Kirkpatrick et al., 1983 ; Dolan et al., 1989). Crystalline structure with a high degree of atomic order is the purest form of the substance, indicating the minimum energy state. The principle of SA mimics the annealing process of slow cooling of molten metal to achieve the minimum function value. The cooling phenomena is simulated by controlling a temperature like parameter introduced with the concept of the Bolzmann probability distribution, which determines the energy distribution probability, P of the system at the temperature, T according to the equation:

$$P(E) = \exp(-E / k_B T_A) \tag{56}$$

where k_B is the Bolzmann constant. The Bolzmann distribution concentrates around the state with the lowest energy. For $T \to 0$, $P(E) \to 0$ and only the state with the lowest energy can have a probability greater than zero. However, cooling the system too fast could result in a higher state of energy and may lead to frozen the system to a metastable state.

The SA is a point by point method based on Monte Carlo approach. The algorithm begins at an initial random point called u and a high temperature T, and the function value at this point is evaluated as $E(k)$. A second point is created in the vicinity of the initial point u and the function value corresponding to this point is obtained as $E(k+1)$. The difference in function values at these points ΔE is obtained as

$$\Delta E = E(k+1) - E(k) \tag{57}$$

If $\Delta E \leq 0$, the second point is accepted, otherwise the point is accepted probabilistically, governed by the temperature dependent Bolzmann probability factor

$$P_r = \exp(-\Delta E / k_B T_A) \tag{58}$$

The annealing temperature, T_A is a parameter in the optimization algorithm and is set by a predefined annealing schedule which starts at a relatively high temperature and steps slowly downward at a prescribed rate in accordance with the equation

$$T_A^{m+1} = \alpha T_A^m, \qquad 0 < \alpha < 1 \tag{59}$$

As the temperature decreases, the probability of the acceptance of the point u will be decreased according to Eq. (58). The parameter α is set such that at the point of convergence, the temperature T_A reaches a small value. The procedure is iteratively repeated at each temperature with the generation of new points and the search is terminated when the convergence criterion set for the objective is met.

Nonlinear modeling and model identification

Various model structures such as Volterra series models, Hammerstein and Wiener models, bilinear models, state affine models and neural network models have been reported in literature for identification of nonlinear systems. Haber and Unbehauen (1990) presented a comprehensive review on these model structures. The model considered in this study for identification of a nonlinear process has a polynomial ARMA structure of the form

$$\begin{aligned}\hat{y}(k) = \theta_0 + \sum_{i=1}^{n_y} \theta_{1,i}\, y(k-i) + \sum_{i=1}^{n_u} \theta_{2,i}\, u(k-i) + \sum_{i=1}^{n_y+1} \theta_{3,i}\, y(k-i)u(k-i) + \\ \sum_{i=1}^{n_u} \sum_{j=1}^{i+1} \theta_{4,ij}\, u(k-i)u(k-j) + ...\end{aligned} \tag{60}$$

or simply

$$\hat{y}(k) = f\left(y(k-1),....., y(k-n_y), u(k-1),....., u(k-n_u)\right) \tag{61}$$

Here k refers the sampling time, y and u are the output and input variables, and n_y and n_u refer the number of output and input lags, respectively. This type of polynomial model structures have been used by various researchers for process control (Morningred et al.,

1992 ; Hernandez and Arkun, 1993). The main advantage of this model is that it represents the process nonlinearities in a structure with linear model parameters, which can be estimated by using efficient parameter estimation methods such as recursive least squares. Thus the model in (61) can be rearranged in a linear regression form as

$$\hat{y}(k) = \theta^T(k-1)\varphi(k-1) + \varepsilon(k) \tag{62}$$

where θ is a parameter vector, φ represents input-output process information and ε is the estimation error. The parameters in the model can be estimated by using recursive least squares based on a priori process knowledge representing the process characteristics over a wide range of operating conditions.

Predictive Model Formulation

The primary purpose of NMPC is to deal with complex dynamics over an extended horizon. Thus, the model must predict the process dynamics over a prediction horizon enabling the controller to incorporate future set point changes or disturbances. The polynomial input-output model provides one step ahead prediction for process output. By feeding back the model outputs and control inputs, the one step-a head predictive model can be recurrently cascaded to itself to generate future predictions for process output. The N step predictions can be obtained as follows

$$\begin{aligned}
\hat{y}(k+1/k) &= f\left(y(k),.....,y(k+1-n_y),u(k),.....,u(k+1-n_u)\right)\\
\hat{y}(k+2/k) &= f\left(\hat{y}(k+1/k),.....,y(k+2-n_y),u(k+1),.....,u(k+M-n_u)\right)\\
\hat{y}(k+N/k) &= f\begin{pmatrix}\hat{y}(k+N-1/k),.....,\hat{y}(k+N-n_y/k),u(k+M-1),.....,\\ u(k+M-n_u)\end{pmatrix}
\end{aligned} \tag{63}$$

where N is the prediction horizon and M is the control horizon.

Objective function

The optimal control input sequence in NMPC is computed by minimizing an objective function based on a desired output trajectory over a prediction horizon:

$$\begin{aligned}
&Min \quad J = \sum_{i=1}^{N}\lambda\left(w(k+i)-\hat{y}_p(k+i)\right)^2 + \sum_{i=1}^{M}\gamma\left(\Delta u(k+i-1)^T\ \Delta u(k+i-1)\right)\\
&u(k),\ u(k+1),.....,u(k+M-1)
\end{aligned} \tag{64}$$

subject to constraints:

$$\begin{aligned}
y_{\min} \le \hat{y}_p(k+i) \le y_{\max} \qquad & (i = 1,.....,N)\\
u_{\min} \le u(k+i) \le u_{\max} \qquad & (i = 0,.....,M-1)
\end{aligned}$$

$$\Delta u_{\min} \le \Delta u(k+i) \le \Delta u_{\max} \qquad (i = 0, \ldots\ldots, M-1)$$

where $\hat{y}_p(k+i)$, i=1, …., N, are the future process outputs predicted over the prediction horizon, w_{k+i}, i=1, …., N, are the setpoints and $u(k+i)$, i=0, ….., M-1, are the future control signals. The λ and γ represent the output and input weightings, respectively. The u_{min} and u_{max} are the minimum and maximum values of the manipulated inputs, and Δu_{min} and Δu_{max} represent their corresponding changes, respectively. Computation of future control signals involves the minimization of the objective function so as to bring and keep the process output as close as possible to the given reference trajectory, even in the presence of load disturbances. The control actions are computed at every sampling time by solving an optimization problem while taking into consideration of constraints on the output and inputs. The control signal, u is manipulated only with in the control horizon, and remains constant afterwards, i.e., $u(k+i) = u(k+M-1)$ for $i = M, \ldots, N-1$. Only the first control move of the optimized control sequence is implemented on the process and the output measurements are obtained. At the next sampling instant, the prediction and control horizons are moved ahead by one step, and the optimization problem is solved again using the updated measurements from the process. The mismatch d_k between the process $y(k)$ and the model $\hat{y}(k)$ is computed as

$$d_k = b(y(k) - \hat{y}(k)) \tag{65}$$

where b is a tunable parameter lying between 0 and 1. This mismatch is used to compensate the model predictions in Eq. (62):

$$\hat{y}_p(k+i) = \hat{y}(k+i) + d_k \qquad (\text{for all } i = 1 \text{ to } N) \tag{66}$$

These predictions are incorporated in the objective function defined by Eq. (64) along with the corresponding setpoint values.

NMPC based on stochastic optimization

NMPC design based on simulated annealing (SA) requires to specify the energy function and random number selection for control input calculation. The control input is normalized and constrained with in the specified limits. The random numbers used for the control input, Δu equals the length of the control horizon, and these numbers are generated so that they satisfy the constraints. A penalty function approach is considered to satisfy the constraints on the input variables. In this approach, a penalty term corresponding to the penalty violation is added to the objective function defined in Eq. (64). Thus the violation of the constraints on the variables is accounted by defining a penalty function of the form

$$P = \sum_{i=1}^{N} \mu \left(\Delta u(k+i)\right)^2 \tag{67}$$

where the penalty parameter, μ is selected as a high value. The penalized objective function is then given by

$$f(x) = J + P \tag{68}$$

where J is defined by Eq. (64). At any instant, the current control signal, u_k and the prediction output based on this control input, $\hat{y}(k+i)$ are used to compute the objective function $f(x)$ in Eq. (68) as the energy function, $E(k+i)$. The $E(k+i)$ and the previously evaluated $E(k)$ provides the ΔE as

$$\Delta E(k) = E(k+i) - E(k) \tag{69}$$

The comparison of the ΔE with the random numbers generated between 0 and 1 determines the probability of acceptance of $u(k)$. If $\Delta E \leq 0$, all $u(k)$ are accepted. If $\Delta E > 0$, $u(k)$ are accepted with a probability of $\exp(-\Delta E/T_A)$. If n_m be the number of variables, n_k be the number of function evaluations and n_T be the number of temperature reductions, then the total number of function evaluations required for every sampling condition are $(n_T \times n_k \times n_m)$. Further details of NMPC based on stochastic optimization can be referred elsewhere (Venkateswarlu and Damodar Reddy, 2008).

Implementation procedure

The implementation of NMPC based on SA proceeds with the following steps.

1. Set T_A as a sufficiently high value and let n_k be the number of function evaluations to be performed at a particular T_A. Specify the termination criterion, ε. Choose the initial control vector, u and obtain the process output predictions using Eq. (63). Evaluate the objective function, Eq. (68) as the energy function $E(k)$.
2. Compute the incremental input vector Δu_k stochastically and update the control vector as

$$u(k+i) = u(k) + \Delta u(k) \tag{70}$$

Calculate the objective function, $E(k+i)$ as the energy function based on this vector.

3. Accept $u(k+i)$ unconditionally if the energy function satisfies the condition

$$E(k+i) \leq E(k) \tag{71}$$

Otherwise, accept $u(k+i)$ with the probability according to the Metropolis criterion

$$\exp\left(-\frac{\left(E(k+i)-E(k)\right)}{T_A^{'}}\right) \geq r \tag{72}$$

where $T_A^{'}$ is the current annealing temperature and r represents random number. This step proceeds until the specified function evaluations, n_k are completed.

4. Carry out the temperature reduction in the outer loop according to the decrement function

$$T_A^{/} = \alpha T_A \tag{73}$$

where α is temperature reduction factor. Terminate the algorithm if all the differences are less than the prespecified ε.

5. Go to step 2 and repeat the procedure for every measurement condition based on the updated control vector and its corresponding process output.

5.2 Case study: nonlinear model predictive control of reactive distillation column

The performance of NMPC based on stochastic optimization is evaluated through simulation by applying it to a ethyl acetate reactive distillation column.

Analysis of Results

The process, the column details, the mathematical model and the control scheme of ethyl acetate reactive distillation column given in Section 3.2 is used for NMPC implementation. In this operation, since the ethyl acetate produced is withdrawn as a product in the distillate stream, controlling the purity of this main product is important in spite of disturbances in the column operation. This becomes the main control loop for NMPC in which reflux flow rate is used as a manipulated variable to control the purity of ethyl acetate. Since reboiler and condenser holdups act as pure integrators, they also need to be controlled. These become the auxiliary control loops and are controlled by conventional PI controllers in which the distillate flow rate is considered as a manipulated variable to control the condenser molar holdup and the bottom flow rate is used to control the reboiler molar holdup. The tuning parameters used for both the PI controllers of reflux drum and reboiler holdups are k_c = - 0.001 and τ_I = 1.99 x 10^4 (Vora and Dauotidis, 2001). The SISO control scheme for the column with the double feed configuration used in this study is shown in the Fig. 3.

The input-output data to construct the nonlinear empirical model is obtained by solving the model equations using Euler's integration with a step size of 2.0 s. A PI controller with a series of step changes in the set point of ethyl acetate composition is used for data generation. The input data (reflux flow) is normalized and used along with the outputs (ethyl acetate composition) in model building. The reflux flow rate is constrained with in the limits of 20 mol/s and 5 mol/s. A total number of 25000 data sets is considered to develop the model. The model parameters are determined by using the well known recursive least squares algorithm (Goodwin and Sin, 1984), the application of which has been shown elsewhere (Venkateswarlu and Naidu, 2001). After evaluating model structure in Eq. (60) for different orders of n_y and n_u , the model with the order n_y=2 and n_u=2 is found to be more appropriate to design and implement the NMPC with stochastic optimization. The structure of the model is in the form

$$\hat{y}_k = \theta_0 + \theta_1 y_{k-1} + \theta_2 u_{k-1} + \theta_3 y_{k-1} u_{k-1} + \theta_4 y_{k-2} u_{k-2} + \theta_5 u_{k-1} u_{k-2} \tag{74}$$

The parameters of this model are determined as θ_0=-0.000774, θ_1=1.000553, θ_2=0.002943, θ_3=-0.003828, θ_4=0.000766 and θ_5=-0.000117. This identified model is then used to derive the future predictions for the process output by cascading the model to it self as in Eq. (63). These model predictions are added with the modeling error, $d(k)$ defined by Eq. (65), which is considered to be constant for the entire prediction horizon. The weightings λ and γ in the objective function, Eq. (64) are set as 1.0 x 10^7 and 7.5 x 10^4, respectively. The penalty parameter, μ in Eq. (67) is assigned as 1.0 x 10^5. The cost function used in NMPC is the penalized objective function, eq. (68), based on which the SA search is computed. The incremental input, Δu in SA search is constrained with in the limits -0.0025 and 0.0025, respectively. The actual input, u involved with the optimization scheme is a normalized value and is constrained between 0 and 1. The objective function in Eq. (68) is evaluated as the energy function at each instant. The initial temperature T is chosen as 500 and the

number of iterations at each temperature is set as 250. The temperature reduction factor, α in Eq. (73) is set as 0.5. The control input determined by the stochastic optimizer is denormalized and implemented on the process. A sample time of 2 s is considered for the implementation of the controller.

The performance of NMPC based on SA is evaluated by applying it for the servo and regulatory control of ethyl acetate reactive distillation column. On evaluating the results with different prediction and control horizons, the NMPC with a prediction horizon of around 10 and a control horizon of around 1 to 3 is observed to provide better performance. The results of NMPC are also compared with those of LMPC presented in Section 3 and a PI controller. The tuning parameters of the PI controller are set as k_C = 10.0 and τ_I = 1.99 x 10^4 (Vora and Dauotidis, 2001). The servo and regulatory results of NMPC along with the results of LMPC and PI controller are shown in Figures 11-14. Figure 11 compares the input and output profiles of NMPC with LMPC and PI controller for step change in ethyl acetate composition from 0.6827 to 0.75. The responses in Figure 12 represent 20% step decrease in ethanol feed flow rate, and the responses in Figure 13 correspond to 20% step increase in reboiler heat load. These responses show the better performance of NMPC over LMPC and PI controller. Figure 14 compares the performance of NMPC and LMPC in tracking multiple step changes in setpoint of the controlled variable. The results thus show the stability and robustness of NMPC towards load disturbances and setpoint changes.

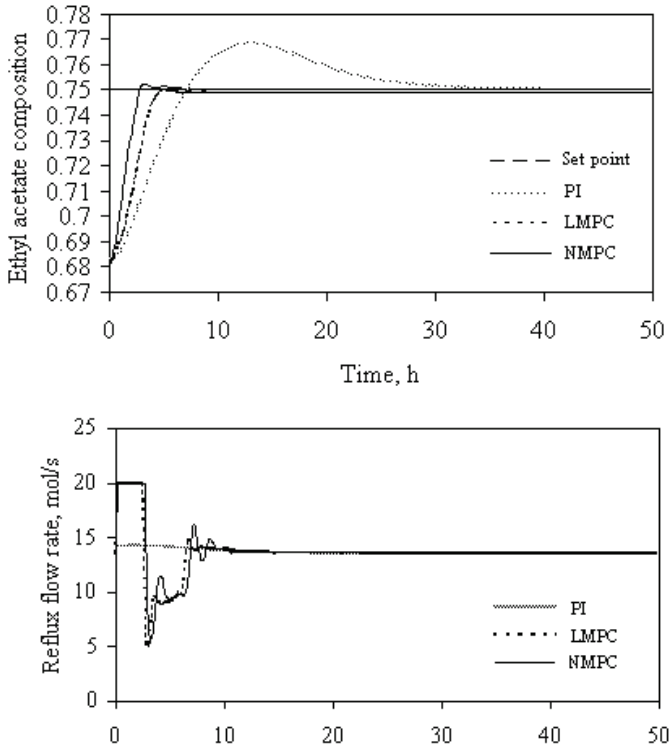

Fig.11. Output and input profiles for step increase in ethyl acetate composition setpoint.

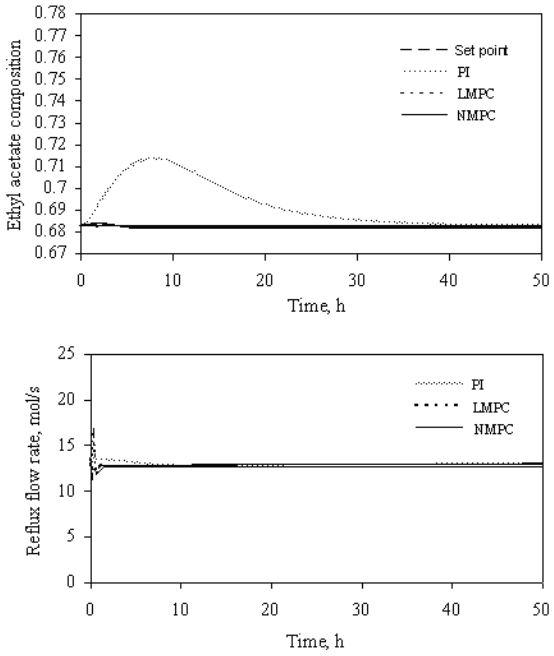

Fig.12. Output and input profiles for step decrease in ethanol feed flow rate.

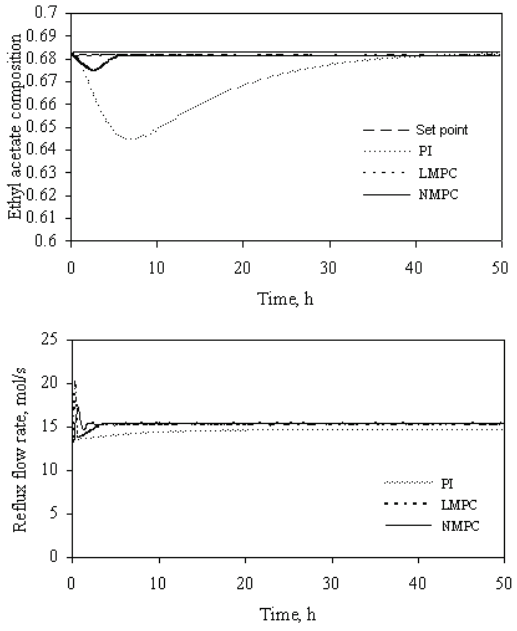

Fig.13. Output and input profiles for step increase in reboiler heat load.

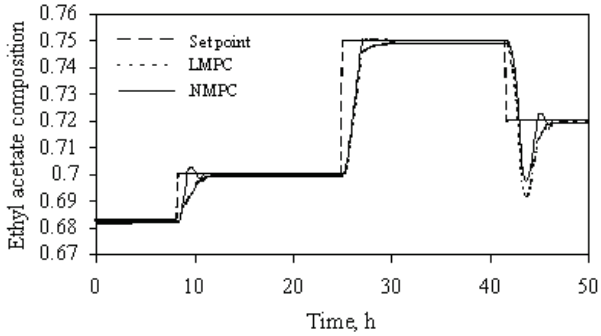

Fig. 14. Output responses for multiple setpoint changes in ethyl acetate composition

6. Conclusions

Model predictive control (MPC) is known to be a powerful control strategy for a variety of processes. In this study, the capabilities of linear and nonlinear model predictive controllers are explored by designing and applying them to different nonlinear processes. A linear model predictive controller (LMPC) is presented for the control of an ethyl acetate reactive distillation. A generalized predictive control (GPC) and a constrained generalized predictive control (CGPC) are presented for the control of an unstable chemical reactor. Further, a nonlinear model predictive controller (NMPC) based on simulated annealing is presented for the control of a highly complex nonlinear ethyl acetate reactive distillation column. The results of these controllers are evaluated under different disturbance conditions for their servo and regulatory performance and compared with the conventional controllers. From these results, it is observed that though linear model predictive controllers offer better control performance for nonlinear processes over conventional controllers, the nonlinear model predictive controller provides effective control performance for highly complex nonlinear processes.

Nomenclature

ARX autoregressive moving average
A_h heat transfer area, m^2
A_{tray} tray area, m^2
B bottom flow rate, mol s^{-1}
B_h dimensionless heat of reaction
C concentration, mol m^{-3}
C_A reactant concentration, mol m^{-3}
C_{Af} feed concentration, mol m^{-3}
C_k catalyst concentration, % vol
C_p specific heat capacity, J kg^{-1} K^{-1}
D distillate flow rate, mol s^{-1}
D_a Damkohler number
du_{min} lower limit of slew rate

du_{max} upper limit of slew rate
E total enthalpy of liquid on plate, kJ
FL liquid feed flow rate on plate, mol s^{-1}
FV vapor feed on plate, mol s^{-1}
F_{Ac} acetic acid feed flow rate, mol s^{-1}
F_{Eth} ethanol feed flow rate, mol s^{-1}
F_o volumetric feed rate, m^3 s^{-1}
H molar enthalpy of vapor stream, kJ mol^{-1}
h molar enthalpy of liquid stream, kJ mol^{-1}
k_1 reaction rate constant, m^3 mol^{-1} s^{-1}
h_{weir} weir height, m
K_C constant of reaction equilibrium
L molar liquid flow rate, mol s^{-1}
L_{weir} weir length, m
L^{liquid} liquid level on tray, m
M molar holdup on plate, m
MW_{av} average molecular weight, g mol^{-1}
N_1 minimum costing horizon
N_2 maximum costing horizon
N_3 control horizon
P pressure on plate, pascal
Q heat exchange, kJ
R number of moles reacted, mol s^{-1}
R_g gas constant, J mol^{-1} K^{-1}
RLS recursive least squares
r rate of reaction, mol s^{-1} m^{-3}
ρ_{av} average density, g m^{-3}
T temperature, K
T_c coolant temperature, K
T_f feed temperature, K
T_r reactor temperature, K
U heat transfer coefficient, J m^{-2} s^{-1} K^{-1}
u controller output
u_{min} lower limit of manipulated variable
u_{max} upper limit of manipulated variable
VLE vapor-liquid equilibrium
V molar vapor flow rate, mol s^{-1}
x mole fraction in liquid phase
x_1 dimensionless reactant concentration
x_2 dimensionless reactant temperature
y mole fraction in vapor phase
y_{min} lower limit of output variable
y_{max} upper limit of output variable
ρ_{av} average density, g m^{-3}

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Phone: +86-21-62489820
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