Multiple Model Predictive Control of a Styrene Polymerization Process

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Abstract. In this paper, multiple piecewise linearizations of a nonlinear process in different operating points are used within a Kalman filter bank which computes the conditional probabilities of various hypotheses that are modeled by the filters. State estimates provided by the Kalman Filters and local model parameters are weighted using conditional probabilities and then used within the predictive control framework. The proposed strategy is tested on the complex model of styrene polymerization process.

1 Introduction

Processes in the chemical industry usually exhibit nonlinear behavior. The nonlinearities arise from the dynamics in chemical reactions, thermodynamic relationships, etc. Such processes are relatively complex and difficult to control. Several methods have been mainly used for predictive control of these processes. The first one is based on the direct use of nonlinear models [1] and involves the online solution of a higher order nonlinear optimization problem with constraints, which is usually computationally expensive and may even be unable to guarantee a feasible solution for real-time control. Another method is to use local linearization approach for representing a nonlinear plant by applying an off-line estimated globally nonlinear and locally linear model to solve a Quadratic Programming (QP) problem online in order to obtain optimal control. A global process model is formed by blending of a number of local models which have been identified over the operating range of the process. Multiple model networks have been more or less independently developed in different disciplines like neural networks, fuzzy logic, statistics and artificial intelligence with different names such as local model networks, Takagi -Sugeno fuzzy models or neuro-fuzzy models [2],[3].

In Continuous Stirred Tank Reactor (CSTR) the product properties are rarely measured accurately on-line, thus much effort has been put to the development of model-based estimation and control techniques. Multivariable nonlinear quadratic dynamic matrix control strategy was applied in [4] to control the polymerization

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process. Both parameter and states of the process are estimated using the Extended Kalman Filters (EKF) and multivariable nonlinear quadratic dynamic matrix control is applied for control of number molecular weight (NAMW). In [5] linear parameter varying (LPV) model which interpolates second order output error models is used to represent the polymerization process. Maner et al. in [6] presented an MPC algorithm based on second-order Volterra models where the model parameters are obtained by discretizing the bilinear Taylor series approximation of the fundamental model. In the paper predictive control is based on a mixture distribution of state-space models [7] with probabilities estimated with a Kalman filter bank.

2 Multiple Model Estimation

The primary feature of Multiple Model Adaptive Estimation (MMAE) is a bank of Kalman filters operating in parallel, using vectors of measurements y and control commands u as their input. Each Kalman filter has the same structure based on the linearized description of the process (Fig. 1). The model is assumed to be linear and of the form:

$$\begin{aligned} \boldsymbol{x}(k+1) &= \boldsymbol{A}\boldsymbol{x}(k) + \boldsymbol{B}\boldsymbol{u}(k) \\ \boldsymbol{y}(k) &= \boldsymbol{C}\boldsymbol{x}(k) + \boldsymbol{D}\boldsymbol{u}(k) \end{aligned} \tag{1}$$

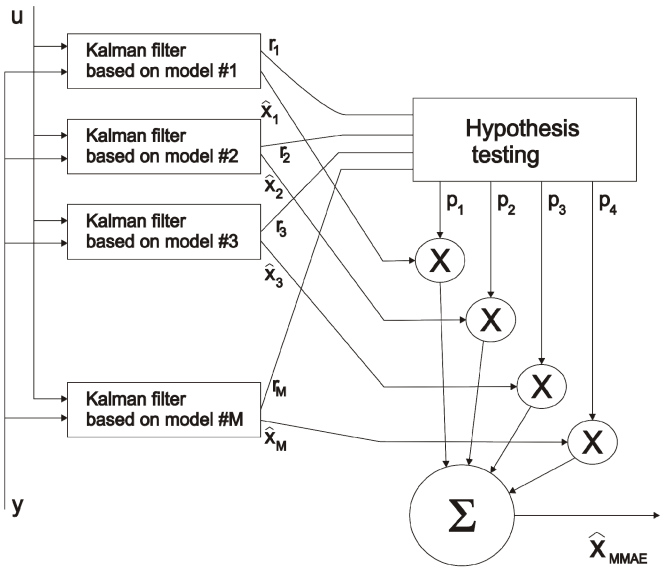

Fig. 1 Multiple Model Adaptive Estimation scheme

Output of each KF is weighted by its corresponding conditional probability based on the measurement history. At every sampling period, each of these Kalman filters is producing its estimate of the state and residual. The idea is that the model with well-behaved residuals contains the parameters that best matches true parameters of the system. Testing the hypothesis which model is the correct one is evaluated in the hypothesis testing block. **T**he initial probability of each hypothesis being correct is distributed evenly:

$$\alpha_i(0) = 1/M \tag{2}$$

The output prediction is given by the mixture of conditional probability density functions:

$$p(y(k)\big|u(k)) = \sum_{i=1}^{M} \alpha_i p_i(y\big(k\big)\big|u(k)) \tag{3}$$

where α_i are the probabilities of each model being the correct one and normalized to 1.

$$\alpha_i = p\big(m(t) = i\big), \sum_{i=1}^{M} \alpha_i = 1 \tag{4}$$

The predictive conditional probability density functions p_i are given by the state-space model as:

$$p_i\left(y\left(k\right)\middle|u\left(k\right)\right) = p_i\left(y(k)\middle|x(k)\right)p_i\left(x(k)\middle|u(k)\right) \tag{5}$$

where $p_i\left(x(k)\middle|u(k)\right)$ is the state-estimate provided by the *i*-th Kalman filter. One step of the Kalman filter can be written as:

$$\begin{aligned} K_i(k) &= A_i P_i(k) C^T \left(I + C_i P_i(k) C_i\right)^{-1} \\ P(k+1) &= A_i P_i(k) A_i + Q_i - K_i\left(C_i P_i(k) C_i + I\right) K_i^T \\ \hat{x}(k+1) &= A_i \hat{x}(k) + B_i u(k) + E_i + \\ &\quad + K_i(y - C_i \hat{x}(k) - D_i u(k) - F_i) \end{aligned} \tag{6}$$

The conditional probability density function for known measurement noise has normal distribution [7] and can be computed using:

$$\begin{aligned} & p(y(k)\big|x(k), \sigma_{ei}^2) = N(y, (1 + C_i P_i C_i^T)\sigma_{ei}^2) \\ & \Sigma = (1 + C_i P_i C_i^T)\sigma_{ei}^2 \\ & p(y(k)\big|x(k), \sigma_{ei}^2) = \frac{1}{(2\pi)^{m/2}\sqrt{|\Sigma|}} \exp\left(-\frac{1}{2}\left(\frac{r_i(k)^T r_i(k)}{\Sigma}\right)\right) \\ & r_i = y(k) - \hat{y}(k) \end{aligned} \tag{7}$$

The estimate of variance can be updated with exponential forgetting with factor φ as:

$$\sigma_{ei}^2(k+1) = \frac{S_i^2(k+1)}{\upsilon(k+1)} \tag{8}$$

where variables S_i^2 and $\upsilon(k+1)$ are updated at each step:

$$\begin{aligned} S_i^2(k+1) &= \varphi\left(S_i^2(k) + \frac{r^T r}{1 + C_i P_i(k+1) C_i} \right) \\ \upsilon(k+1) &= \varphi(\upsilon(k)+1) \end{aligned} \tag{9}$$

3 Description of the Styrene Polymerization Process

The proposed control strategy is tested on the model of the free radical solution polymerization of styrene in a jacketed CSTR. The reactor is controlled around the low conversion stable steady-state point. Two controlled variables are considered: number average molecular weight (y_1) and reactor temperature (y_2). The initiator flow (u_1) and the cooling flow rate (u_2) were selected as manipulated variables. This work uses a mathematical model of the styrene polymerization process shown in Fig. 2. The nonlinear process is modeled by the following differential equations:

$$\begin{aligned} \frac{d[I]}{dt} &= \frac{\left(Q_i[I_f] - Q_t[I]\right)}{V} - k_d[I] \\ \frac{d[M]}{dt} &= \frac{\left(Q_m[M_f] - Q_t[M]\right)}{V} - k_d[M][P] \\ \frac{dT}{dt} &= \frac{Q_t\left(T_f - T\right)}{V} + \frac{\left(-H_r\right)}{\rho C_p} k_p[M][P] - \frac{hA}{\rho C_p V}\left(T - T_c\right) \\ \frac{dT_c}{dt} &= \frac{Q_c\left(T_{cf} - T_c\right)}{V_c} + \frac{hA}{\rho C_{pc} V_c}\left(T - T_c\right) \\ \frac{dD_0}{dt} &= 0.5 k_t[P]^2 - \frac{Q_t D_0}{V} \\ \frac{dD_1}{dt} &= M_m k_p[M][P] - \frac{Q_t D_1}{V} \\ u_1 = Q_i, u_2 = Q_c, y_1 &= \frac{D_1}{D_0}, y_2 = T \end{aligned} \tag{10}$$

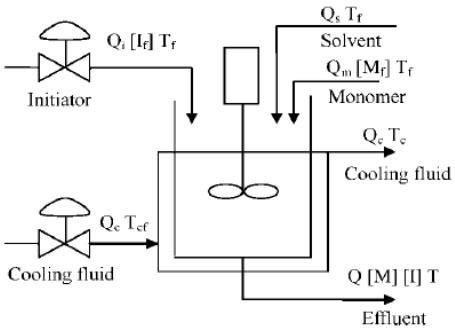

Fig. 2 CSTR reactor

where the rate constants are given as:

$$k_i = A_i \exp\left(-E_i / T\right), i = d, p, t$$
$$\left[P\right] = \sqrt{\frac{2fk_d\left[I\right]}{k_t}}, Q_t = Q_i + Q_s + Q_m \tag{11}$$

The goal of the control system is to drive the polymerization system to a new state to produce polymers with different number average molecular weights while keeping the temperature at its setpoint. The kinetic parameters and thermodynamic parameters can be found in [5].

4 State-Space Predictive Control

The state-space model based predictive control is based on the time-invariant model:

$$\begin{aligned} x(k+1) &= \boldsymbol{A}x(k) + \boldsymbol{B}u(k) \\ y(k) &= \boldsymbol{C}x(k) + \boldsymbol{D}u(k) \end{aligned} \tag{12}$$

The model of the process is obtained at every sampling interval and its parameters are used for the entire prediction horizon *Hp*. The discrete model contains also the affine part that results from linearization around non-zero steady-state:

$$\begin{aligned} &x(k+1) = \boldsymbol{A}x(k) + \boldsymbol{B}u(k) + \boldsymbol{E} \\ &y(k) = \boldsymbol{C}x(k) + \boldsymbol{D}u(k) + \boldsymbol{F} \\ &\boldsymbol{A} = \sum_{i=1}^{M} p_i \boldsymbol{A}_i, \boldsymbol{B} = \sum_{i=1}^{M} p_i \boldsymbol{B}_i, \boldsymbol{E} = \sum_{i=1}^{M} p_i \boldsymbol{E}_i \\ &\boldsymbol{C} = \sum_{i=1}^{M} p_i \boldsymbol{C}_i, \boldsymbol{D} = \sum_{i=1}^{M} p_i \boldsymbol{D}_i, \boldsymbol{F} = \sum_{i=1}^{M} p_i \boldsymbol{F}_i \end{aligned} \tag{13}$$

The H_p -step ahead output prediction can be deduced:

$$\begin{aligned}
&\hat{\boldsymbol{Y}} = \Phi_{yx}\boldsymbol{x}(k) + \Phi_{yu}\boldsymbol{U} + \Phi_{y0} \\
&\hat{\boldsymbol{Y}} = \begin{bmatrix} \hat{y}(k+1) \\ \hat{y}(k+2) \\ \vdots \\ \hat{y}(k+H_p) \end{bmatrix}, \boldsymbol{U} = \begin{bmatrix} u(k) \\ u(k+1) \\ \vdots \\ u(k+H_p) \end{bmatrix}, \Phi_{yx} = \begin{bmatrix} \boldsymbol{CA} \\ \boldsymbol{CA}^2 \\ \vdots \\ \boldsymbol{CA}^{H_p} \end{bmatrix} \\
&\Phi_{yu} = \begin{bmatrix} \boldsymbol{CB} & \boldsymbol{D} & 0 & 0 & 0 \\ \boldsymbol{CAB} & \boldsymbol{CB} & \boldsymbol{D} & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \boldsymbol{CA}^{H_p-1}\boldsymbol{B} & \boldsymbol{CA}^{H_p-2}\boldsymbol{B} & \cdots & \boldsymbol{CB} & \boldsymbol{D} \end{bmatrix} \\
&\Phi_{y0} = \begin{bmatrix} \boldsymbol{CE} + \boldsymbol{F} \\ \boldsymbol{CAE} + \boldsymbol{CE} + \boldsymbol{F} \\ \vdots \\ \boldsymbol{CA}^{H_p-1}\boldsymbol{E} + \ldots + \boldsymbol{CE} + \boldsymbol{F} \end{bmatrix}
\end{aligned} \tag{14}$$

The computation of a control law of MPC is based on minimization of the following criterion:

$$J_{MPC} = \left(\hat{\boldsymbol{y}} - \boldsymbol{w}\right)^T \boldsymbol{Q}\left(\hat{\boldsymbol{y}} - \boldsymbol{w}\right) + \Delta\boldsymbol{u}\boldsymbol{R}\Delta u \tag{15}$$

where $\hat{y}(k+j|k)$ is a j steps ahead prediction of the system, $w(k+j)$ is a future reference trajectory and $\boldsymbol{Q}, \boldsymbol{R}$ are positive definite weighting matrices. The minimization of the criterion can be transformed into a quadratic programming problem:

$$J_{MPC} = \boldsymbol{u}^T \boldsymbol{H}\boldsymbol{u} + \boldsymbol{f}\boldsymbol{u} \tag{16}$$

where matrix H and vector f are derived from model parameters given by (14)equation reference goes here. The quadratic problem is usually solved numerically. As formulated, the nonlinear model predictive controller will exhibit steady – state offset in the presence of plant/model mismatch due to a lack of integral action. To introduce an integral action to remove steady-state error an integrator state must be added to the system:

$$\begin{aligned}
&v(k) = v(k-1) + (w(k) - y(k)) \\
&\xi(k) = \begin{bmatrix} x(k) \\ v(k) \end{bmatrix}
\end{aligned} \tag{17}$$

System matrices (12) are updated as follows:

$$\begin{aligned}
&\xi(k+1) = \tilde{\boldsymbol{A}}\xi(k+1) + \tilde{\boldsymbol{B}}u + \tilde{\boldsymbol{E}} \\
&y(k) = \tilde{\boldsymbol{C}}\xi(k+1) + \tilde{\boldsymbol{D}}u + \tilde{\boldsymbol{F}} \\
&\tilde{\boldsymbol{A}} = \begin{bmatrix} \boldsymbol{A} & 0 \\ -\boldsymbol{C} & \boldsymbol{I} \end{bmatrix}, \tilde{\boldsymbol{B}} = \begin{bmatrix} \boldsymbol{B} \\ -\boldsymbol{D} \end{bmatrix}, \tilde{\boldsymbol{E}} = \begin{bmatrix} \boldsymbol{E} \\ \boldsymbol{W}(k) - \boldsymbol{F} \end{bmatrix} \\
&\tilde{\boldsymbol{C}} = \begin{bmatrix} \boldsymbol{C} & 0 \end{bmatrix}, \tilde{\boldsymbol{D}} = \boldsymbol{D}, \tilde{\boldsymbol{F}} = \boldsymbol{F}
\end{aligned} \tag{18}$$

In order to minimize the augmented state the cost criterion for MPC (22) is transferred to:

$$J_{MPC} = \left(\hat{\boldsymbol{Y}} - \boldsymbol{W}\right)^T \boldsymbol{Q}\left(\hat{\boldsymbol{Y}} - \boldsymbol{W}\right) + \Delta \boldsymbol{U}^T \boldsymbol{R} \Delta \boldsymbol{U} + \hat{\boldsymbol{X}}^T \boldsymbol{S} \hat{\boldsymbol{X}} \tag{19}$$

where

$$\hat{\boldsymbol{X}} = \Phi_{xx} \boldsymbol{x}(k) + \Phi_{xu} \boldsymbol{U} + \Phi_{x0} \tag{20}$$

$$\Phi_{xx} = \begin{bmatrix} \boldsymbol{A} \\ \boldsymbol{A}^2 \\ \mathsf{M} \\ \boldsymbol{A}^{H_p} \end{bmatrix}, \Phi_{x0} = \begin{bmatrix} \boldsymbol{E} \\ \boldsymbol{A}\boldsymbol{E} + \boldsymbol{E} \\ \mathsf{M} \\ \boldsymbol{A}^{H_p - 1}\boldsymbol{E} + \ldots + \boldsymbol{E} \end{bmatrix}$$
$$\Phi_{xu} = \begin{bmatrix} \boldsymbol{B} & 0 & 0 & 0 & 0 \\ \boldsymbol{A}\boldsymbol{B} & \boldsymbol{B} & 0 & 0 & 0 \\ \mathsf{M} & \mathsf{M} & \mathsf{O} & \mathsf{O} & \mathsf{M} \\ \boldsymbol{A}^{H_p - 1}\boldsymbol{B} & \boldsymbol{A}^{H_p - 2}\boldsymbol{B} & \mathsf{L} & \boldsymbol{B} & 0 \end{bmatrix} \tag{21}$$

5 Implementation

Multiple-model predictive control described in Section 4 is applied for control of the NAMW and temperature of CSTR. Three linear models were obtained through linearization in steady-state operating points for input signals $u_1 = 72{,}108$ and 144 l/h. The sampling period was set to 1h due to the dynamics of the process. In practice the NAMW is measured with sampling period of 30 minutes and the time delay of the measurement is also 30 minutes. The Kalman filter bank with these local models was constructed with initial condition $x = \begin{bmatrix} 0.0784 \\ 3.3516 \\ 324.9078 \\ 305.6496 \\ 0.0004 \\ 19.4179 \end{bmatrix}$ which corresponds to the third operating point. The initial estimate covariance matrix was chosen to be:

$$P = 10^4 I \tag{22}$$

and saturation constraints in the manipulated variables are imposed to take into account the minimum/maximum aperture of the valve regulating the flow rates. The prediction horizon was set to 20 samples as a result of using different values

and comparing control performances. The weighting matrices Q,R,S associated with the error from set-point, control output increment and integrator gain were set to:

$$Q = \begin{bmatrix} 0.0001 & 0 \\ 0 & 100 \end{bmatrix}, R = \begin{bmatrix} 10 & 0 \\ 0 & 10 \end{bmatrix}, S(7,7) = 0.01, S(8,8) = 100 \tag{23}$$

The results of a closed-loop simulation for a set-point changes from 51 494 to 64 463 g/mol which corresponds to operating point #3 and #2 are shown in Fig. 3, where they are compared with the results obtained from the linear MPC controller and the nonlinear MPC controllers without the integral behavior. At t= 150h an disturbance is introduced by increasing the value of monomer flow-rate by 10%. model. The linear model is only valid in the vicinity of the operating point #3 and as the system is driven out this point the steady-state error increases. If both models of the system at the operating points are available and the current model is identified by Kalman filters correctly (Fig. 4) then the zero steady state-error can be obtained at the operating point #2. However, the system is not able to cope with the disturbance that is not included in the model. Zero off-set is reached when multiple models also contain augmented state.

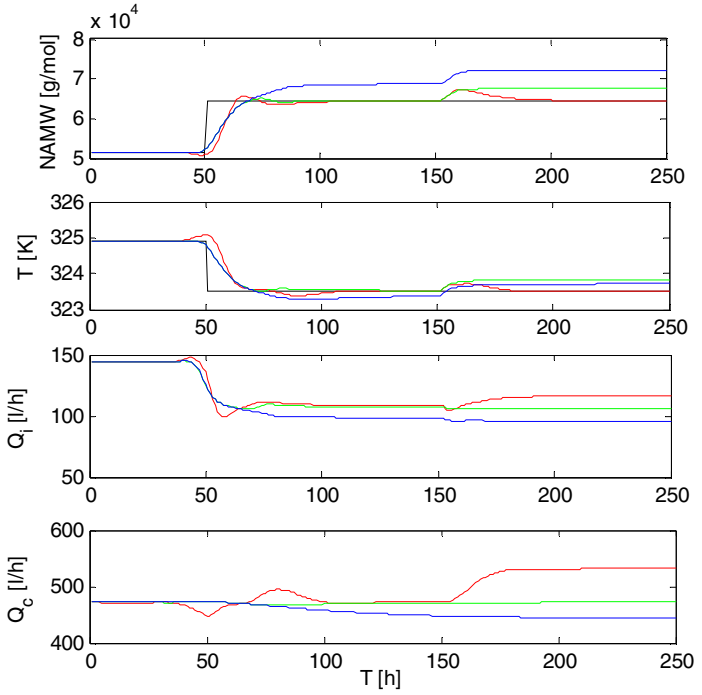

Fig. 3 Closed loop simulation for transition control (black – reference, blue – linear MPC with single model, green - Multiple model MPC, red - Multiple model MPC with integrator state)

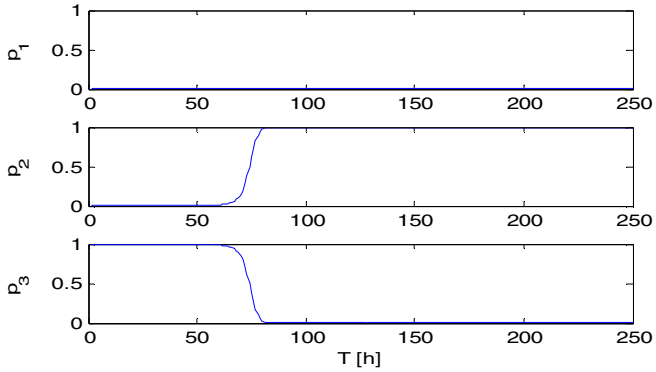

Fig. 4 Probability of each of the model during the closed loop simulation

6 Conclusion

In the paper, a multiple-model predictive control methodology is applied to a styrene polymerization system. The correct model at the current sampling point is estimated using the residuals provided by a bank of Kalman filters. The obtained state is in the form of a mixture of states provided by the filters. The parameter of the linearized model and the states are then used within the predictive control approach for prediction of the future plant behavior. To remove steady-state error for model/plant mismatch an augmented state is added to the state space description. The simulations show that this type of predictive control can be applied to the styrene polymerization system effectively.

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