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Nonlinear Model Predictive Control of Chemical Reactors

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Abstract

A robust nonlinear predictive control strategy using a disturbance estimator is presented. The disturbance estimator is comprised of two parts: one is the disturbance model parameter adaptation and the other is future disturbance prediction. RLSM(recurrsive least square method) with a forgetting factor is used to determine the uncertain disturbance model parameters and for the future disturbance prediction, future process outputs and inputs projected by the process model are used. The simulation results for chemical reactors indicate that a substantial improvement in nonlinear predictive control performance is possible using the disturbance estimator.

Introduction

It is well recognized that a characteristic of chemical processes that presents a challenging control problem is the inherent nonlinearity of the process. During the past decade, linear model predictive control techniques have been greatly developed and well received by industry because they are intuitive and explicitly handle constraints. But one of the limitations to the existing linear model predictive control strategies are that they are based on linear systems theory and may not perform well on highly nonlinear systems. Several approaches for nonlinear predictive control were presented. There are two representive nonlinear predictive methods. One method uses the linearized model of nonlinear differential equations and its control law is same as linear model predictive control(Li and Biegler, 1989; Brengel and Seider, 1989; Gutta and Zafiriou). The other method is a nonlinear programming approach that uses a nonlinear optimization code such as GRG(Generalized Reduced Gradient) and SQP(Successive Quadratic Programming) to calculate the control law(Bequette, 1991; Patwardhan and Edgar,1990). All these approaches are incorporated with parameter identification algorithm to get good control performance and robustness. So most of nonlinear control strategies have assumed that all state variables are measured or are easily estimated. But if the number of state variables are far more than that of measurements, estimation of all the states and parameters may be difficult or meaningless. Even when all of the state variables are measured or estimated, the control performance may not be satisfactory if there are model structure errors. So it is necessary to make the nonlinear predictive control strategies robust without depending on process model parameter identification algorithms.

In this study, a new approach is developed to deal with model/plant mismatch or unknown disturbances. This approach combine the Newton-type controller(Li and Biegler, 1989) with a disturbance estimator. We used RLSM(Recurrsive Least Square Method) with the forgetting factor to estimate uncertain parameters of the disturbance model where all available process inputs and output measurements are needed. Using the disturbance model, future disturbances can be projected with present process inputs and output measurements remaining constant in the prediction horizon and future process inputs are calculated based on the process outputs prediction including them. And then for the more accurate disturbance prediction, the future disturbances are recalculated with primarily calculated process inputs and predicted process outputs to get better process output predicton. This step is repeated until the difference between the projected and the prior projected future disturbances becomes sufficiently small. The nonlinear predictive control with the disturbance estimator has some merits as follows :

● It is robust for the processes with severe model uncertainty.

● It shows good control performance because future process inputs are recalculated based on accurate disturbance prediction.

● The disturbance estimator may be independently used from a nonlinear model parameter identification algorithm.

● It is effective when the model structure is changed or the number of state variables is far more than that of measurements.

Review of Nonlinear Model Predictive Control

The nonlinear predictive control problem is typically formulated as follows :

$$min\ \Phi(u) = \int_{t0}^{tf} e(t)^2 dt = \sum_{i=k}^{k+P} [y_{sp}(i) - y_{pred}(i)]^2 \qquad (1)$$

subject to

$$\frac{dx}{dt} = f(x,u) \qquad (2)$$

$$y = g(x) \qquad (3)$$

$$y_{min} \le y \le y_{max} \qquad (4)$$

$$u_{min} \le u \le u_{max} \qquad (5)$$

$$x(t0) = x0 \qquad (6)$$

In nonlinear programming approach, orthogonal collocation on finite elements is used to transfer the differential equation into a set of algebraic equations, then the above objective function can be expressed as a function of future process inputs and solved directly with a nonlinear optimization code such as GRG(Generalized Reduced Gradient) and SQP(Successive Quadratic Programming) to calculate the control law(Bequette, 1991; Patwardhan and Edgar,1990). In linear approximation approach, differential equations are linearized, and arranged as a function of a set of future process inputs, then we can apply QP(Quadratic Programming) to the above control problem and get a set of future process inputs. Only first process input is applied to the process and at the next sampling time all the calculation are repeated(Li and Biegler, 1989; Brengel and Seider, 1989; Gatta and Zafiriou).

Disturbance Estimator

Linear model predictive control are always consistent because the difference between predicted process outputs and measurements is interpreted as being due to additive disturbances. Of course, in linearized model based nonlinear predictive control, the above concept can be used to compensate the difference caused by model/plant mismatch or unknown disturbances. However, since unknown disturbances or model/plant mismatch can profoundly influence the process outputs in nonlinear processes, it is far better to get the information about how disturbances actually influence the process and add the predicted disturbances to process output prediction than to simply add the difference between model outputs and measurements.

In NLQDMC(Nonlinear Quadratic Dynamic Matrix Control), the disturbance vector $d(k)$ is defined that $y_m(k)$ - $y(k)$, where $y_m(k)$ is a measurement vector. It is added to the process output prediction directly under the assumption of $d(k+i) = d(k)$ for $i = 1, 2, ...P$ where P is the prediction horizon. So such assumption may cause unexpected results under severe model/plant mismatch in nonlinear processes.

In the multistep Newton-type Controller(Li and Biegler, 1989), A primary limitation of the technique is that a perfect model is assumed; they suggested that an on-line parameter estimation technique should be added to update the model. But when the number of state variables is far more than that of measurements or the model structure is changed, the technique may not work well. After all, their method totally depends on on-line model parameter identification techniques to remove steady-state offset when there are model/plant mismatch or unknown disturbances.

Parrish and Browsilow(1988) developed NLIC (Nonlinear Inferential Control) to estimate unmeasured disturbances and follow a desired setpoint trajectory. Their method does not account for state variable constraints and can not handle systems, of which the process gains change signs in the operating region (Bequette, 1991).

In order to resolve all those difficulties, we add a disturbance estimator to the multistep Newton-type controller. Of course, NLQDMC can be used instead of the multistep Newton-type controller because both of them are based on linearized models. The disturbance estimator consists of two parts , one is disturbance model parameter adaptation using RLSM with the exponential forgetting factor, the other is future disturbance prediction using the disturbance model. The basic algorithm for disturbance estimation is as follows :

● Disturbance model parameter adaptation

A linear discrete model is used for disturbance model parameter adaptation as follows.

$$d(k) = \phi^T \theta \qquad (7)$$

where

$\theta = [a_1 a_2 \ldots a_n \quad b_1 b_2 \ldots b_n]$

$\phi = [y_m(k) \; y_m(k-1) \ldots y_m(k-n) \quad u(k) \ldots u(k-n)]$

Here, n is the order of process model outputs and inputs in the disturbance model equation. How to determine n is not clear, but the bigger n is generally the better the performance of model adaptation is. RLSM with the exponential forgetting factor is good for the model parameter adaptation of slowly time-varying processes. Since the disturbance model is a unknown nonlinear system, we can use RLSM with the exponential forgetting factor under the assumption that the disturbance model is time-varying. RLSM with the exponential forgetting factor(Å strom, 1989) is as follows:

$$\hat{\theta}(k) = \hat{\theta}(k-1) + K(k)(d(k) - \phi^T\hat{\theta}(k-1)) \quad (8)$$

$$K(k) = P(k)\phi(k) = P(k-1)\phi(k)(\lambda I + \phi(k)P(k-1)\phi(k))^{-1} \quad (9)$$

$$P(k)^{-1} = P(k-1)^{-1} + \phi(k)\phi(k)^T \quad (10)$$

where $\hat{\theta}(k)$: estimated parameter vector

Here, we suggest a linear discrete model as the disturbance model. If a bilinear model is used, the regression vector ϕ would be changed as $[y_m(k)\; y_m(k-1) \ldots y_m(k-n)\; y_m(k)u(k)\; y_m(k-1)u(k-1) \ldots y_m(k-n)u(k-n)\; u(k)\; u(k-1) \ldots u(k-n)]$. Later, we compare the control performance between the linear and the bilinear disturbance model.

● Disturbance prediction

step 1 : Start with output measurements $y_m(k)$, model outputs $y(k)$, and process inputs $u(k)$.

step 2 : Set $d(k) = y_m(k) - y(k)$ and calculate the predicted disturbances $d_{pred}(i)$ with $y(i) = y_m(k)$ and $u(i) = u(k)$ for $i = k+1, k+2, \ldots k+P$.

step 3 : Solve $min\ \Phi(u) = \sum_{i=k+1}^{k+P} [y_{sp}(i) - y_{pred}(i) - d_{pred}(i)]^2$

s.t. equations (2) - (4)

Through this step, future inputs $u(i)$ for $i = k+1, k+2, \ldots, k+P$ are calculated and for the convenience, let these values $u_{old}(i)$.

step 4 : Recalculate the predicted disturbances; $d_{pred}(i)$ with future process inputs; $u_{old}(i)$, and $d(k)+y(i)$ where $y(i)$ are the future model outputs calculated with these future process inputs.

The reason why $d(k)$ is added to $y(i)$ is to give more approximated process output prediction since the predicted output by model equations only can not be exact.

step 5 : Set $diff(i) = d^2_{pred}(i) - d^1_{pred}(i)$ where superscript 1 and 2 are old and newly calculated predicted disturbances respectively in step 4. Solve

$$min\ \Phi(\Delta u) = \sum_{i=k+1}^{k+P} [diff(i)]^2$$

s.t. $u_{min} \le u_{old}(i) + \Delta u(i) \le u_{max}$

step 6 : If $\sum \| diff(i) \| < \varepsilon$ where ε is a sufficiently small number, then set $u_{new}(i) = u_{old}(i) + \Delta u(i)$ as ultimate process inputs and go to step 1. Otherwise, set $d^1_{pred}(i) = d^2_{pred}(i)$, $u_{old}(i) = u_{old}(i) + \Delta u(i)$, and go to step 4.

Examples and Simulation

An adiabatic CSTR with an exothermic, first order irreversible reaction is used as a SISO nonlinear process. The resulting model equation is as follows;

$$\frac{dx_1}{dt} = -\alpha x_1 \exp\left(\frac{x_2}{1 + x_2/\gamma}\right) + q(x_{1f} - x_1)$$

$$\frac{dx_2}{dt} = -\beta \alpha x_1 \exp\left(\frac{x_2}{1 + x_2/\gamma}\right) - (q+\delta)x_2 + \delta x_3 + qx_{2f}$$

where x_1 is the dimensionless concentration, x_2 is the dimensionless temperature(controlled variable), x_3 is the dimensionless cooling jacket temperature(manipulated variable), and the subscript 'f' means feed. The nominal parameter values are shown in Table 1 (Limqueco and Kantor, 1990; Bequette, 1991)

Table 1. Model parameter values and initial conditions

Model parameters & initial conditions	value
α	0.072
β	8
δ	0.3
γ	20.0
x_{1f}	1.0
x_{2f}	0.0
x_{3f}	0.0

Under the nominal parameter values, this system has three states, The lower- and upper-temperature steady states are stable, while the middle temperature steady state is unstable.

To know how robust the NTC(Newton-Type controller) with a disturbance estimator is, we apply the technique to the system when one of the model parameter value, $\delta = 0.3$ is changed to 3.0. In the case, the steady-state operating curve according to δ is greatly changed as shown in figure 1 since there is no sign change. So we can say that the extent of model/plant mismatch is severe. For the simulation of control performance, the process is assumed to behave the original process model equation(δ =0.3) while the model for the design of Newton-type controller depends on δ =3.0. We assume the concentration x_1 is measured and the process input, u is bounded between -1 and 2. Figure 2 shows the control performances of NTC, NTC with additive disturbance, and NTC with a disturbance estimator for a setpoint change to the open-loop unstable point x_1=0.5528, x_2=2.7517. As expected, the NTC without the model parameter identification shows steady-state offset, and NTC with additive disturbance oscillates periodically around the setpoint. However, NTC with the disturbance estimator shows good control performace without any steay-state offset.

Figure 3 shows the results when the model parameter, δ is changed to 0.12. The NTC with a disturbance estimator shows good control performance while the others are oscillationg around the setpoint. The prediction horizon in which the model output is to match the desired trajectory is an important tuning parameter for nonlinear predictive control techniques. Generally the larger prediction horizon is, the better control performance is. But in the case of model/plant mismatch, long prediction horizon may result in bad control action and performance. Figure 4 shows the comparison between NTC(P=1) and multistep NTC(P=5) with a disturbance estimator. The multistep NTC caused the steady-state offset. That is because the predicted disturbance values are oscillated and the total predicted error sum goes to zero. Therefore, the prediction horizon should be chosen to be as short as possible to minimize the errors introduced by projecting the disturbance into the future in the case of model/plant mismatch. We used the 4th order linear disturbance model for all simulation studies. A bilinear model for the disturbance can give the better result than the linear model. Figure 5 shows the control performance of NTC with a disturbance estimator using the 4th order bilinear model. The design of NTC is based on δ = 3.0 and after 30 time steps, δ =0.3 in the process is changed to 0.2. The process input is bounded between -2 and 2. NTC using a bilinear disturbnace model shows the shorter settling time. Even when x1 is unmeasured, there is little change for the control performance (Figure 6). Therefore, the disturbance model which can represent the nonlinearity of unknown disturbance closely is required to get good control performance and robustness.

Conclusions

Nonlinear model predictive control using the disturbance estimator shows good control performance and robustness. It is found that RLSM with an exponential forgetting factor is good as a disturbance model parameter adaptation algorithm and the better future disturbance prediction is possible with it than with the assumption that present differences between measurements and model outputs are constant over all prediction horizon. The concept of disturbance estimator can be expanded to other nonlinear predictive control techiques without much modification. Also, it may be used independently with process model parameter identification techniques and is easily added to the existing nonlinear predictive control strategies. It is especially effective when the model stucture is changed or the number of state variable is far more than that of measurements.

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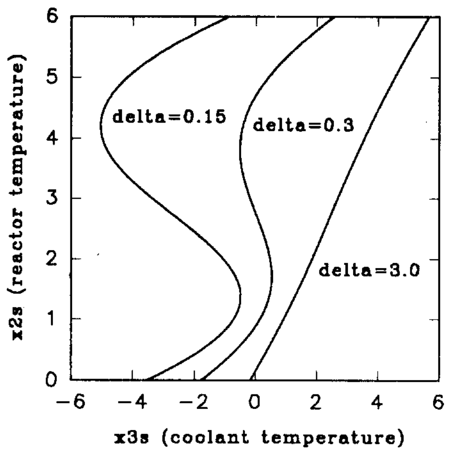

Figure 1. Sensitivity of the steady-state operating curve to δ.

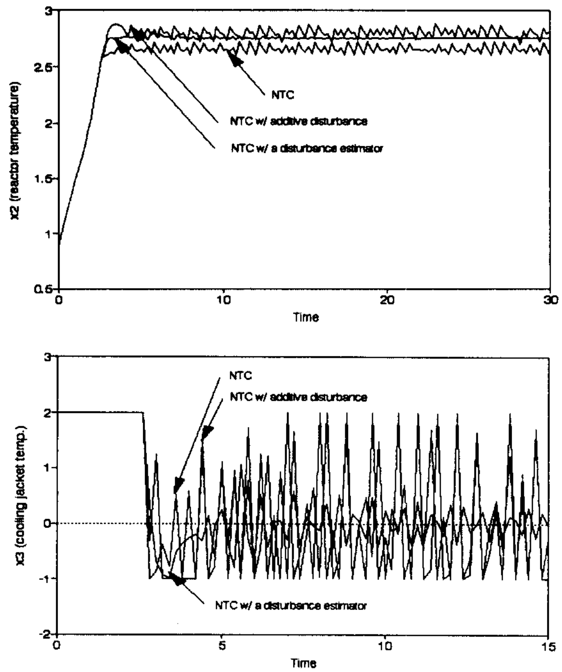

Figure 3. Setpoint change to unstable operating point with model uncertainty(plant δ=0.3, model δ=0.12).

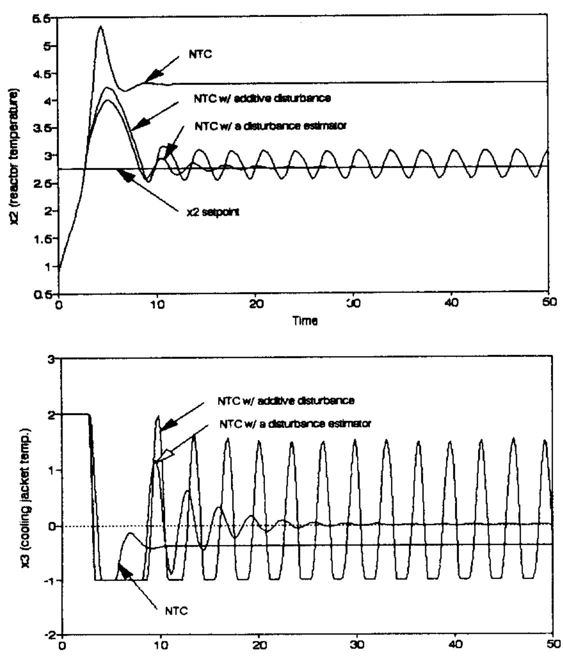

Figure 2. Setpoint change to unstable operating point with model uncertainty(plant δ=0.3, model δ=3.0).

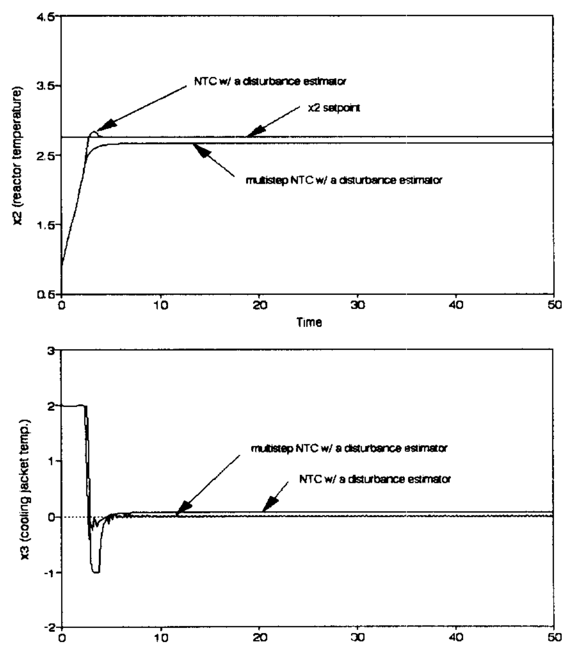

Figure 4. Comparison of the control performance between NTC(P=1) and multistep NTC(P=5).

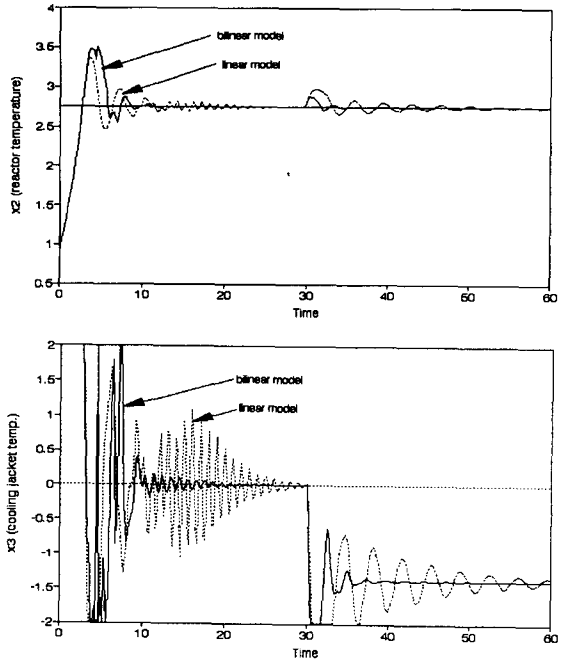

Figure 5. Comparison of the control performance between the linear and the bilinear disturbance model.

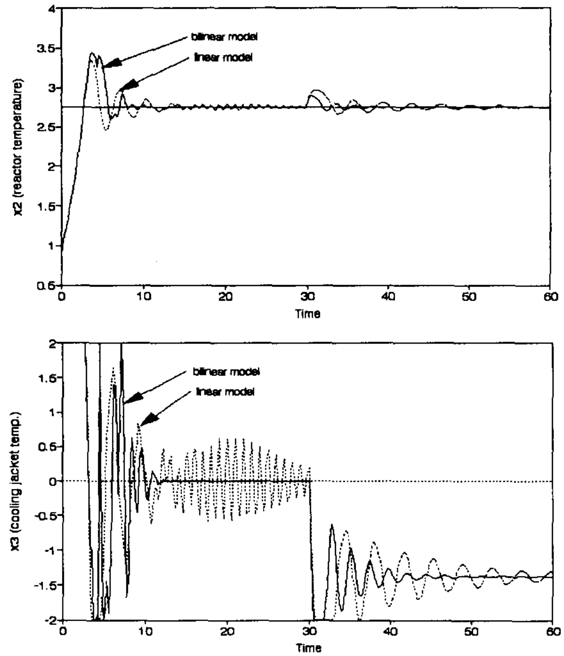

Figure 6. Comparison of the control performance between the linear and the bilinear disturbance model(x_1 is unmeasured).