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SHORT COMMUNICATION

Model Predictive Control for the Reactant Concentration Control of a Reactor

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Abstract–The reactant concentration control of a reactor using Model Predictive Control (MPC) is presented in this paper. Two major difficulties in the control of reactant concentration are that the measurement of concentration is not available for the control point of view and it is not possible to control the concentration without considering the reactor temperature. Therefore, MIMO control techniques and state and parameter estimation are needed. One of the MIMO control techniques widely studied recently is MPC. The basic concept of MPC is that it computes a control trajectory for a whole horizon time minimising a cost function of a plant subject to a dynamic plant model and an end point constraint. However, only the initial value of controls is then applied. Feedback is incorporated by using the measurements/estimates to reconstruct the calculation for the next time step. Since MPC is a model based controller, it requires the measurement of the states of an appropriate process model. However, in most industrial processes, the state variables are not all measurable. Therefore, an extended Kalman filter (EKF), one of estimation techniques, is also utilised to estimate unknown/uncertain parameters of the system. Simulation results have demonstrated that without the reactor temperature constraint, the MPC with EKF can control the reactant concentration at a desired set point but the reactor temperator is raised over a maximum allowable value. On the other hand, when the maximun allowable value is added as a constraint, the MPC with EKF can control the reactant concentration at the desired set point with less drastic control action and within the reactor temperature constraint. This shows that the MPC with EKF is applicable to control the reactant concentration of chemical reactors.

Key words: Model Predictive Control, Kalman Filter, Reactor

INTRODUCTION

An optimisation model based feedback controller design known as "Model Predictive Control (MPC)" technique has been required to handle highly nonlinear chemical processes including constraints. The basic idea of MPC is to determine a set of controls for a whole time horizon by minimising a cost function of the plant subject to a dynamic plant model incorporating plant nonlinearities, and an end point constraint. The initial value of control is then applied to the plant.The use of measurements/estimates of state and repeating the calculation provides feedback controls action. It has been shown theoretically that, under restricted conditions, this approach guarantees plant stabilisation. Kwon and Pearson [1977], Mayne and Michalska [1990], and Kershenbaum et al. [1993] have derived the stabilising properties of the MPC in several systems.

The control performance of the MPC technique has been widely tested in several systems for over a decade. First of all, the MPC technique was applied together with neural network structure in pH control which involved significant nonlinearity and uncertainty. Simulation results showed that the MPC controller with the neural network gave satisfactory control response [Warwick et al., 1992].

Secondly, the MPC strategy was tested in the control of a simulated gas sweetening unit. The control objective was to regulate the output of the modelled unit (the partial pressure of the carbon-dioxide at the output gas stream) to a set point value of 0.001 bar by means of manipulating mono-ethanolamine (M.E.A.) solution and steam flows. The performance of the MPC was compared to that of open loop optimal control. It was found that the MPC gave better control response than the optimal control did. Control results showed the success of the MPC in handling both disturbances and moderate modelling errors. Nonetheless, the steady state offset could not be eliminated; the MPC could not provide any kind of an integral control action [Grbovic, 1992].

Extended work on controlling the gas sweetening unit was carried out based on more realistic models. The main goal was to keep the process output below a specified level, not to stabilise the unit. Simulation results showed that the MPC was able to account for a large disturbance reasonably well [Kershenbaum et al., 1993].

The application of the MPC on an exothermic batch reactor was addressed by eg. Kittisupakorn and Ruksawid [1998]. It was found that the MPC could control the temperature of the batch reactor, which involved highly nonlinear behaviour and subjected to constraints, at a desired set point and gave a better control performance than the PID did. In the presence of plant/model mismatch, the EKF was incorporated in the MPC to estimate unknown/uncertain parameters. As a result, the MPC with EKF was robust; it could give good control performance in the presence of plant/model mismatch.

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The control of a continuous stirred tank reactor using the MPC technique has been widely studied by eg. Patwardhan et al. [1990], Sistu and Bequette [1991] and Ramamurthi et al. [1993]. However, such study has aimed to control the temperature rather than the reactant concentration of the reactor. On the other hand, to set up product specifications, the reactant concentration needs to be controlled rather than the reactor temperature. The control of reactant concentration faces two major difficulties. The first one is that it is not possible to control the concentration without considering the reactor temperature due to safety reasons. The other one is that the measurement of concentration is not available for the control point of view. Therefore, this paper is aimed to study the reactant concentration control of a CSTR using the MPC with an extended Kalman filter with respect to the difficulties.

DESCRIPTION OF A CONTINUOUS REACTOR

The reactor used by Limqueco and Kantor [1990] has been studied here. This system consists of a jacketed CSTR in which a first order, irreversible reaction, $A \xrightarrow{k_o} B$, takes place. Assumptions made in formulating the model are: the reactor is perfectly mixed and no heat loss occurs within the system, the amount of heat retained in the reactor walls is negligible, all temperatures are measurable, the jacket temperature can be directly manipulated without delay i.e. the cooling water jacket dynamics can be neglected and the feed concentration is assumed to be a known constant in this case.

Under the assumptions above, the energy and mass balances in the CSTR can be written as follows:

$$\frac{dTr}{dt}=\frac{(-\Delta H)}{\rho Cp}k_o Ca e^{\frac{-E}{RTr}}+\frac{F}{Vr}(Tf-Tr)+\frac{UrAr}{\rho CpVr}(Tj-Tr) \tag{1}$$

$$\frac{dCa}{dt}=-k_o Ca e^{\frac{-E}{RTr}}+\frac{F}{Vr}(Cao-Ca) \tag{2}$$

The meaning of letters and symbols are given in Nomenclature. The physical properties and process data are given in Table 1.

The main purpose of this simulation study is to evaluate the performance of the MPC with estimator to control the reactant concentration (Ca) of the reactor to a desired steady state by adjusting the jacket temperature (Tj) with/without a reactor temperature constraint.

Tabel 1. Physical properties and process data for the experimental study

$Ur=68.0$ kcal/(min·m^2 °C)	$k_0=3.64*10^6$ min^{-1}
$Ar=0.7$ m^2	$\Delta H=8000.0$ kcal/kmol
$Vr=0.24$ m^3	$E/R=6000.0$ °K^{-1}
$Cpr=Cpj$ kcal/(kg^3 °C)	$F=0.0036$ m^3/min
$Cpj=1.0$ kcal/(kg·°C)	$Tj=293.15$ K (20 °C)
Initial steady state condition	
$Ca(0)=5.364$ kmol/m^3	$Tr(0)=333.15$ K (60 °C)
$Cao=25.0$ kmol/m^3	$Ca_{sp}=5.364$ kmol/m^3
$Tfo=300.15$ K (23 °C)	

THEORETICAL DESCRIPTION

1. Model Predictive Control

The basic concept of the Model Predictive Control (MPC) is that it calculates future controls based on current measurements via the solution of an optimal control problem but only the first element of controls is applied to the process. Then, the states are measured or estimated and used as initial conditions in order to recalculate the future controls by re-solving the optimal control problem.

1-1. Optimal Control Problem

In this work, the reactant concentration of the reactor is controlled at a desired set point by adjusting the jacket temperature (without considering the control cost). Therefore, the optimal control problem can be given by a cost function (Performance Index):

$$\min\int_0^{t_f} W(Ca-Ca_{sp})^2 dt \tag{3}$$

where W is a weighting factor.

Subject to the system equations (Eqs. (1) and (2)), a final state constraint (Eq. (4)), a bounded control (Eq. (5)) and a reactor temperature constraint (Eq. (6))

$$(Ca-Ca_{sp})(t_f)=0 \tag{4}$$

$$293.15\le Tj(t)\le 333.15 \tag{5}$$

$$Tr(t)\le 338.15 \tag{6}$$

with the initial conditions (Eqs. (7) and (8)) and time horizon (Eq. (9))

$$Tr(0)=333.15 \tag{7}$$

$$Ca(0)=5.364 \tag{8}$$

$$0\le t\le 20. \tag{9}$$

The objective function (Eq. (3)) is included to define that the reactant concentration is controlled to a desired set point minimising the error between the control response and the set point for a whole time horizon. It should be noted that in several control problems the control action movement is also included in the objective function. However, since the main goal of this work is to control the reactant concentration with respect to the reactor constraint (Eq. (6)) for safety reasons, the inclusion of the control action movement in the objective function is not considered. In addition, to ensure that the reactant concentration is forced to a desired set point at the terminal time (t_f) [Mayne, 1995], Eq. (4) is included.

To find the solution of the optimal control problems, FROTRAN programmes, based on the optimisation algorithm described by Pytlak and Vinter [1992], have been written for solving the problems with terminal equality and inequlity constraints and with constraints on states and controls. Terminal equlity constraints are tackled by an exact penalty function. A second order correction step is applied to equality constraints. Simple control constraints are tackled by a projection which leads to a fast recognition of active control constraints at a solution. The inequality constraints are treated through a feasible direction approach. A direction of descent is obtained by solving a convex optimal

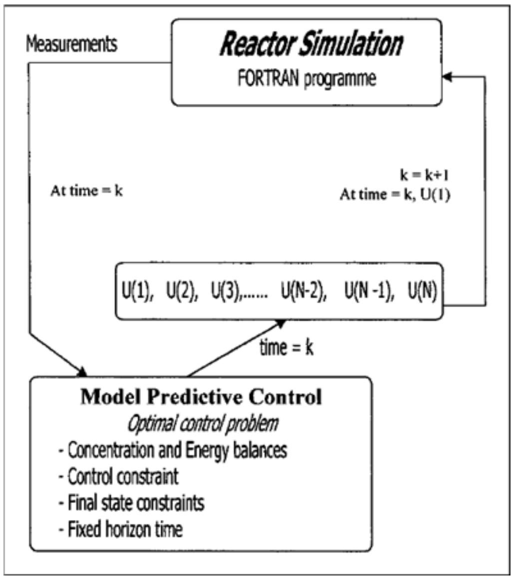

Fig. 1. Information flowchart of the MPC algorithm.

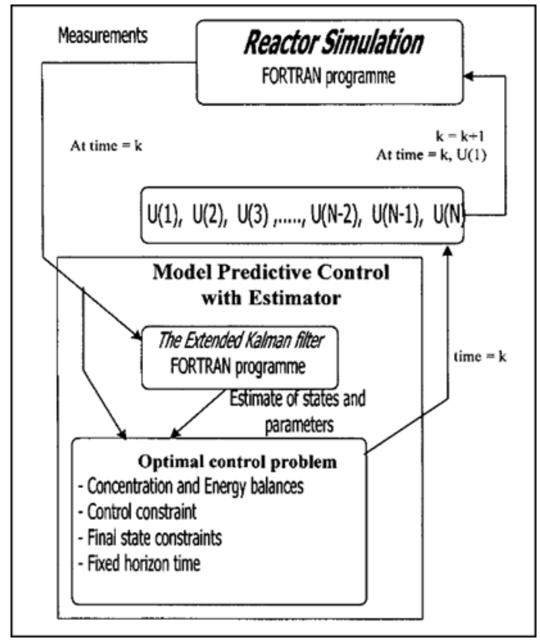

Fig. 2. Information flowchart of the MPC with EKF.

control problem by means of quadratic programming procedure.

Fig. 1 illustrates the information flowchart of the MPC algorithm. A control trajectory U(k) (referring to Tj(k)) for an entire horizon is computed on-line based on current states. The initial value of controls is then implemented to the system, which means that the control action at time k+1 is the control U(1) (referring to Tj(1)) of future controls calculated at time k. Some feedback is provided by measurements of state at the next interval and repeating the calculation. In other words, measurements are compared to a set point or predicted value so that the error between the measurements and a set point can be utilised within the MPC algorithm. The MPC algorithm, then, produces the future controls which minimise this error.

2. Model Predictive Control (MPC) with Estimator

The MPC technique provides control actions based upon reference models. However, in practice, the measurement of the reactant concentration may not be available. Therefore, the estimates of concentration are needed. Here, the extended Kalman filter (EKF) described by e.g. Meybeck [1982] is applied to estimate the reactant concentration on-line using the available measured temperature.

For the purposes of estimation, the state equations for the reactor are: from energy and material balances of the reactor, (Eqs. (1) and (2)). The EKF tuning parameters: $\hat{P}$, Q and R, are tuned to reflect the accuracy of estimation of unmeasured reactant concentration. Table 2 shows the values of the EKF tuning parameters: $\hat{P}$, Q and R and initail state estimates for the EKF.

Fig. 2 illustrates the flowchart of the MPC with the EKF approach. As we see from the MPC algorithm, a set of control actions is determined on-line based on current states. Only the first element of controls is applied to the system; the control action at time k+1 is the control U(1) (referring to Tj(1)) of future controls calculated at time k. Some feedback is obtained by measurements of state at the next interval and repeating the calculation. The inclusion of the EKF is for estimating the unmeasured state X_2 (referring to Ca) using the available measurement of X_1 (referring to Tr). Measurements and estimates are compared to a set point or predicted value. As a result, the error between the measurements and set point or predicted value caused by plant/model mismatch or disturbances can be utilised within the MPC algorithm. The MPC algorithm, then, produces the future controls which minimise this error based on the updated model parameters.

Table 2. Filter parameters and initial state estimates for simulation studies

$X_1(0)=333.15$ K	$\hat{P}_{11}=1.0$	$Q_{11}=9.0$
$X_2(0)=5.364$ kmol/m^3	$\hat{P}_{22}=0.3$	$Q_{22}=4.0$
$R_{11}=0.05$		

CONTROL IMPLEMENTATION

1. Case Study

The main purpose of this simulation study is to evaluate the performance of the MPC algorithm. Here, the MPC algorithm [with/without the reactor temperature constraint (Eq. (6))] has been studied to control the reactant concentration to a desired set

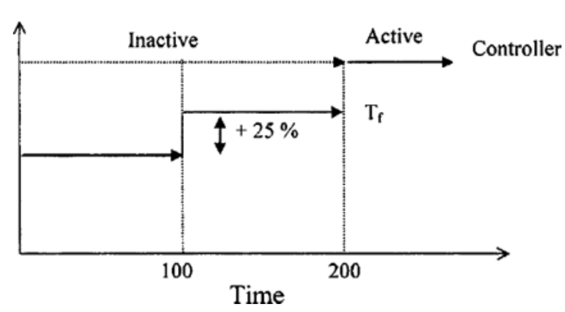

Fig. 3. Case study (a step disturbance in feed flowrate).

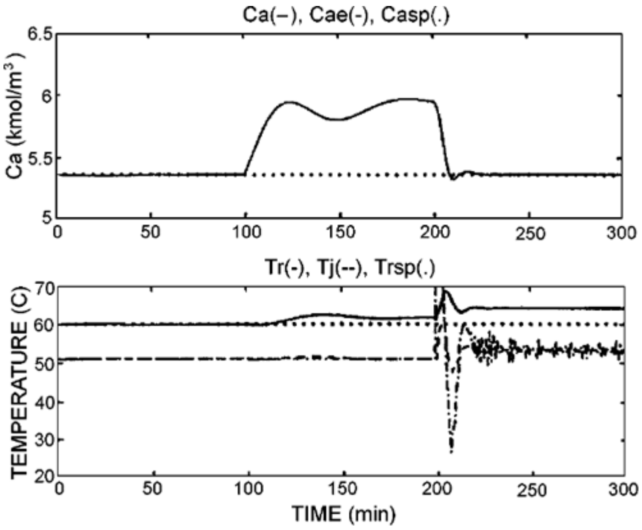

Fig. 4. Response of the MPC with EKF.

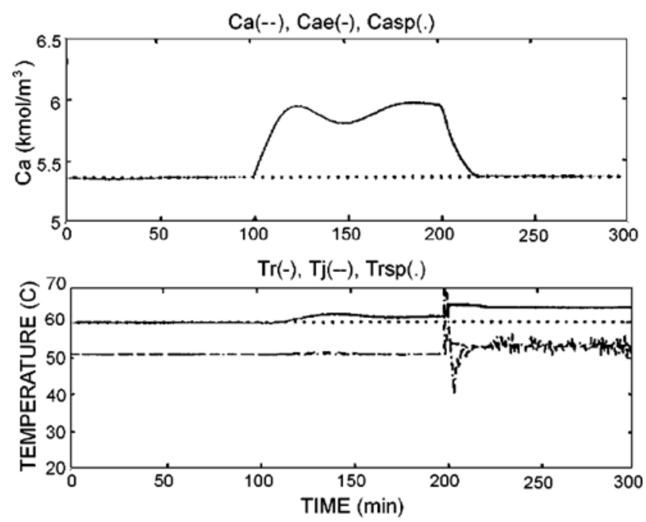

Fig. 5. Response of the MPC with EKF subject to the reactor temperature constraint.

point by adjusting the jacket temperature. The reactor is simulated from an initial conditions until a feed flowrate disturbance (25% increase form the nominal case) is introduced at time = 100 minutes and is kept throughout the simulation. Then the MPC is activated at time = 200 minutes. Fig. 3 illustrates the case study.

2. Simulation Results

To achieve the main goal, here, the weighting factor W is chosen to be 10.

Figs. 4 and 5 show the control performances of the MPC with EKF with and without the reactor temperature constraint repectively. It can be seen that without the reactor temperature constraint, the MPC with EKF can bring the reactant concentration quickly back to the desired set point with a small overshoot. As expected, to bring the reactant concentration back to the set point as quickly as possible, the reactor temperature needs to be raised quickly; it goes beyond the maximum allowable value (65 °C). Then, it is reduced and settled at about 64 °C and the

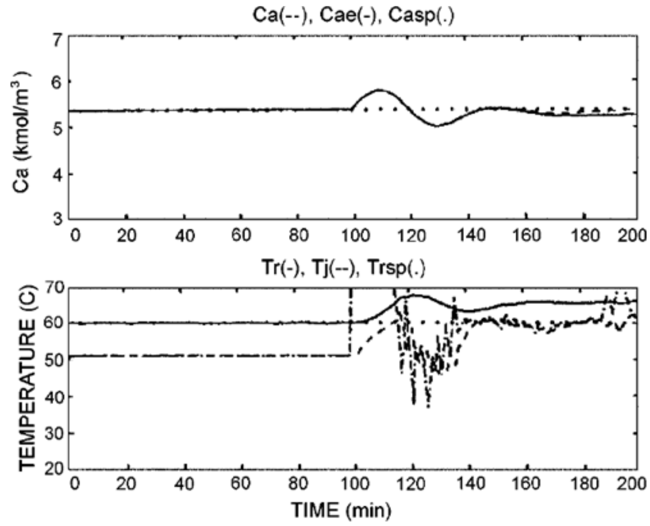

Fig. 6. Response of the MPC with EKF subject to the reactor temperature constraint in the presence of mismatch in heat transfer coefficient.

reactant concentration is stable at the set point.

On the other hand, without any change in MPC or EKF parameters, the MPC with the EKF subject to the reactor temperature constraint gives control actions to quickly raise the reactor temperature up too. However, since the reactor temperature constraint is included, the reactor temperature cannot be increased over the constraint. Therefore, the reactant concentration takes longer time to reach the set point than the previous result. In other words, the MPC with EKF can control the reactant concentration at the desired set point with less drastic control action and within the reactor temperature. This result demonstrates that the MPC algorithm can handle state constraints of the system constraint.

3. Robustness Test

The MPC algorithm with EKF has been tested in the presence of plant/model mismatch in the heat transfer coefficient (20% increase) and the rate constant (20% increase) and with the reactor temperature constraint. It was found that althought the mismatches have been included, the MPC with EKF can still control the reactant concentration at the set point and within the reactor temperature constraint. This result ensures that the MPC with EKF is able to control the reactant concentration of chemical reactors without any violation of safety concerns.

CONCLUSIONS

The Model Predictive Control (MPC) with Extended Kalman Filter (EKF) with/without state constraints has been studied here. In this work, the MPC with EKF has been applied to control the reactant concentration of a reactor. Simulation results have demonstrated that without the reactor temperature constraint, the MPC with EKF can control the reactant concentration at a desired set point but the reactor temperator is raised over a maximum allowable value. On the other hand, when the maximun allowable value is added as a constraint, the MPC with EKF can control the reactant concentration at the desired set point with less drastic control action and within the reactor temperature constraint. In addition, in the presense of plant/model mismatches in the heat transfer coefficient and the rate constant, the MPC with EKF can still produce good control response; the reactant concentration is controlled at the set point and within the reactor temperature contraint. This shows that the MPC with EKF is applicable to control the reactant concentration of chemical reactors.

NOMENCLATURE

A	: component "A"
Ar	: heat transfer area [m^2]
B	: component "B"
Ca	: reactant concentration [$kmol/m^3$]
Cao	: nominal feed concentration [$kmol/m^3$]
Cp	: specific heat capacity [kcal/(kg·C)]
E	: activation energy [kcal/kmol]
F	: volumetric flowrate [m^3/min]
Fo	: nominal volumetric flowrate [m^3/min]
ΔH	: heat of reaction [kcal/kmol]
k_0	: Arrhenius pre-exponential constant [min^{-1}]
P, Q	: EKF parameters
R	: universal gas constant [kcal/(kmol·K)]/EKF parameters
t	: time [Min]
Tr	: reactor temperature [K]
Tj	: jacketed temperature [K]
Tf	: feed temperature [K]
U	: manipulated variables
Ur	: heat transfer coefficient [kcal/(s·m^2·C)]
Vr	: volume of reactor [m^3]
X	: state variables

Greek Letter

ρ	: reactant density [kg/m^3]

Subscipts

a	: component "A"
c	: cooling water
f	: feed condition
o	: initial condition or nominal condition
sp	: set point

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