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AN INVESTIGATION ON MODEL PREDICTIVE CONTROLLERS' APPLICATIONS OF A CHEMICAL ENGINEERING PROCESS

M.Sc. Thesis by

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Department : Chemical Engineering

Programme: Chemical Engineering

JUNE 2006

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JUNE 2006

İSTANBUL TEKNİK ÜNİVERSİTESİ ★ FEN BİLİMLERİ ENSTİTÜSÜ

MODEL ÖNGÖRÜLÜ KONTROL EDİCİLERİN KİMYA MÜHENDİSLİĞİ PROSESLERİNE UYGULANMASI ÜZERİNE BİR ÇALIŞMA

YÜKSEK LİSANS TEZİ

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Emre Özgen Kuzu

May 2006

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NOMENCLATURE

AMPC	: Adaptive Model Predictive Controller
CARIMA	: Controlled Auto Regressive Integrated Moving Average
CARMA	: Controlled Auto Regressive Moving Average
CSTR	: Continuous Stirred Tank Reactor
DMC	: Dynamic Matrix Control
DMC-plus	: Dynamic Matrix Control Plus
EKF	: Extended Kalman Filter
GLC	: Globally Linearizing Control
GPC	: Generalized Predictive Control
HEICON	: Hierarchical Constraint Control
IDCOM	: Identification & Command
IDCOM-M	: Identification & Command - Multi
IMC	: Internal Model Control
LMPC	: Linear Model Predictive Control
LQG	: Linear Quadratic Gaussian Control
MAC	: Matrix Algorithmic Control
MIMO	: Multi Input – Multi Output
MPC	: Model Predictive Control
MPHC	: Model Predictive Heuristic Control
NLPC	: Nonlinear Predictive Control
NMPC	: Nonlinear Predictive Control
QDMC	: Quadratic Dynamic Matrix Control
QP	: Quadratic Programming
SISO	: Single Input – Single Output
SMCA	: Setpoint Multivariable Control Architecture
SMOC	: Shell Multivariable Optimizing Controller
SVD	: Singular Value Decomposition

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LIST OF SYMBOLS

F_A	: Flow rate of propylene oxide and methanol mixture
F_B	: Flow rate of water
F_{CW}	: Flow rate of coolant, water
C_{Ai}	: Initial concentration of propylene oxide entering the reactor
C_{Bi}	: Initial concentration of water entering the reactor
C_{Mi}	: Initial concentration of methanol entering the reactor
C_{Ci}	: Initial concentration of propylene glycol the reactor
CV	: Controlled Variables
V	: Volume of the reactor
T_i	: Initial temperature of feed streams
T_{a1}	: Initial temperature of coolant
k_r,	: Reaction rate constant
E	: Activation energy
R	: The gas constant
Cp	: Heat Capacity
ΔH_{rxn}	: Heat of reaction
ρ	: Density
MD	: Measured Disturbance
MV	: Manipulated Variable
MW	: Molecular weight of coolant
UA	: Heat transfer coefficient * Heat transfer area
UD	: Unmeasured Disturbance
a	: Step response Coefficient
C	: Control Horizon
E	: Closed loop prediction error
E'	: Open loop prediction error
H	: Hessian matrix
M	: Model horizon
n	: Current step time
P	: Prediction horizon
u	: Process input
W	: Weighting matrix
Δ	: Increment
Λ	: Diagonal element of weighting matrix

MODEL ÖNGÖRÜLÜ KONTROL EDİCİLERİN KİMYA MÜHENDİSLİĞİ UYGULAMALARIÜZERİNE BİR ARAŞTIRMA

ÖZET

Model öngörülü kontrol ediciler, bir sisteme ait modeli kullanarak bir öngörü ufku boyunca gelecek çıktı değerlerini hesaplayarak gelecekteki hataları en aza indirecek kontrol sinyallerini hesaplar. Doğrusal olmayan ya da parametreleri zamanla değişebilen sistemlerde kullanılabilmesi, ölü zamanlı sistemlere uygunluğu, gürbüzlüğü ve kullanım kolaylığı Model Öngörülü Kontrol algoritmasının en önemli avantajlarıdır.

Bu çalışmada, Model Öngörülü Kontrol edicilerin kimya mühendisliğinin en öenmli uygulamalarından biri olan kimyasal reaktörlerde kullanımı ve performansı incelenmiştir. Propilen oksit ve su reaksiyonundan ortaya çıkan propilen glikolun konsantrasyonu ve reaktörün sıcaklığı, propilen oksit ve soğutma suyunun akış debisinin ayarlanması ile control edilmiş, soğutma suyu sıcaklığı ve propilen oksitin giriş konsantrasyonu bozucu etki olarak değerlendirilmiştir.

Tasarlanan kontrol edici, ayar noktası değişimleri ve bozucu etkilere karşı cevabı yönünden incelenmiştir. Bu etkilere kontrol edicinin kısa sürede cevap verdiği gözlemlenmiştir. Ayrıca kontrol edicinin gürbüzlüğünü test etmek amacı ile sistem parametreleri değiştirilmiş ve kontrol edicinin yeni sistemde de o modele ait olmayan basamak cevabı ile reaktörü kontrol edebildiği gözlemlenmiştir.

AN INVESTIGATION ON MODEL PREDICTIVE CONTROLLERS' APPLICATIONS OF A CHEMICAL ENGINEERING PROCESS

SUMMARY

Model predictive controllers calculate the control signals to minimize future errors by calculating future output values in a prediction horizon by using a model of the system. Successful applications to nonlinear systems, parametric uncertainties, dead time compensation, its robustness and ease of use are the main advantages of Model Predictive Control algorithm.

In this study, applications and performance of MPC on chemical reactors, one of the most important chemical engineering applications, are examined. Propylene glycol concentration, resulting from reaction of propylene oxide and water, is controlled with reactor temperature by manipulating propylene oxide and coolant flow rates. Temperature of cooling water and initial concentration of propylene oxide are evaluated as measured disturbances.

The designed controller is examined in terms of set point tracking and disturbance rejection. It is seen that the controller tracks the set point and rejects the effect of disturbances in a reasonably short time. Also in order to test the robustness of the controller, the system parameters have been changed and it is observed that the controller performs finely with old step response data model.

1. INTRODUCTION

The chemical industry can be characterized as stable for redesign considerations, since economic factors prevent new design considerations. On the other hand the industry, especially petrochemical industry exhibits very dynamic market place conditions (Garcia et al.,1989). Under these circumstances, effective control structures acts as an important player for success and profit in the industry.

Garcia et al. (1989) describes that success can be achieved by the integration of all aspects of automation of the decision making process. This integration must include process measurements via instrumentation, control of systems; analog and rapid sampling digital controllers for auxiliary systems and high capacity controls for multivariable plans with large computational capacities. Control of the systems must be followed by optimization step in which manipulation of process for economic and other concerns or constraints. Finally the allocation of raw materials and scheduling of operating plants must be organized in coordination with previous actions.

It is a fact that in practice the operating point of a plant that satisfies the overall economic goals of the process will lie at the intersection of the constraints (Arkun, 1978). Economic, safety and environmental, equipment, product quality and human preferences are the main constraints that a controller must handle. Garcia et al. 1978 suggests that Model Predictive Control (MPC) techniques provide the only methodology to handle the constraints in a systematic way during the design and the implementation of the controller.

MPC is defined as a class of control algorithms "in which there is a direct use of an explicit and separately identifiable model (Prett and Garcia, 1988). Muske and Rawlings (1993) suggested a more detailed description as "MPC refers to the class of control algorithms that compute a manipulated input profile by utilizing a process model to optimize an open loop performance objective subject to constraints over a future time horizon".

MPC is an open code with certain principles which allow for future extensions rather than a strict structure. This flexibility brings a variety of advantages applicable to many industries and needs. Camacho and Bordons (1999) listed the advantages of MPC compared to other control techniques as:

- It is particularly attractive to staff with limited knowledge, since the concepts are intuitive and tuning is relatively easy.
- It is applicable to a great variety of processes, from those with relatively simple dynamics to more complex ones, including systems with long delay times or of non-minimum phase or unstable ones.
- The multivariable case can easily be dealt with.
- It has compensation for dead times.
- It introduces feed forward control in a natural way to compensate for measurable disturbances
- The resulting controller is an easy to implement linear control law.
- Its extension to the treatment of constraints is conceptually simple and these can be systematically included during the design process.
- It is very useful when future references are known.

In this study, MPC application and performance will be investigated on one of the most important figures in chemical industry, chemical reactors. As a case study, production of ethylene glycol from the reaction of ethylene oxide-methanol mixture and water in a continuous stirred tank reactor, CSTR. The controller design necessitates development of system model which shows a nonlinear behavior. Multi-input multi - input (MIMO) based MPC is developed, where the temperature of the reactor and concentration of product, ethylene glycol, is being controlled by manipulating ethylene oxide and coolant flow rates with presence of coolant temperature and water flow rates as measured disturbances.

The performance of the controller is analyzed for set point tracking, disturbance rejection and robustness.

2. LITERATURE SURVEY

2.1 A Brief History of MPC

Although Model Predictive Control (MPC) originated in the late seventies, the theory behind dates back to 1950s and 1960s with the concept of using an open-loop optimal control computation as in MPC case. However implementations of the theory become possible with the sudden increase in the computational power.

MPC describes a class of computer control algorithms that control the future behavior of a plant through the use of an explicit process model (Qin and Badgwell, 2003). Based on this basic definitions and approaches, several industrial MPC algorithms have been developed and are shown in Figure 2.1.

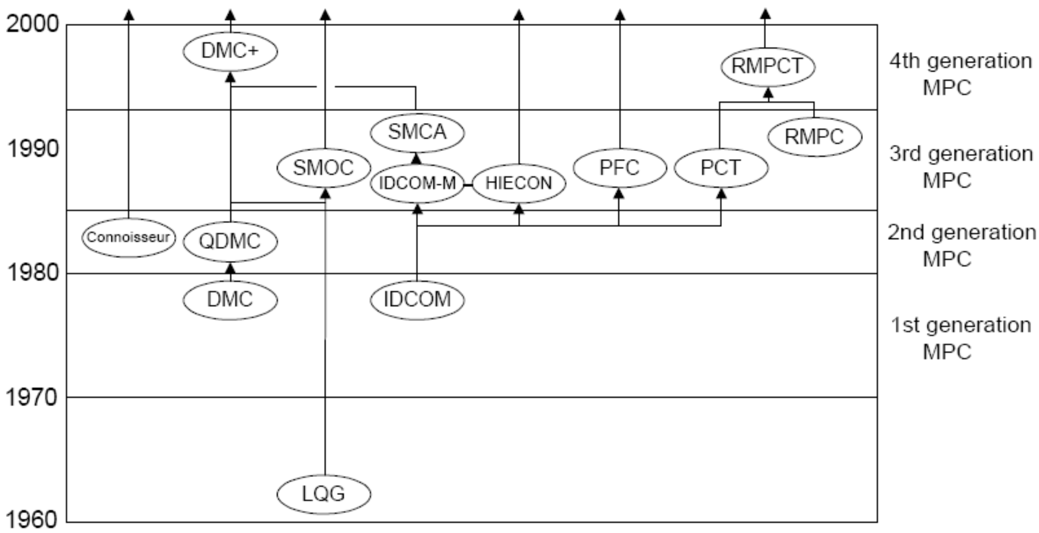


Figure 2.1 : Historical development of MPC algorithms, (Qin and Badgwell, 2003)

2.1.1 Linear Quadratic Gaussian Control (LQG)

The idea behind MPC can be traced back to works by Kalman in the early 1960s on Linear Quadratic Gaussian (LQG) control (Qin and Badgwell, 2003). LQG concept is based on the formulation of the system by a discrete-time, linear state space model. State disturbances and measurement noises are also added to that model. These inputs were assumed to be Gaussian noise with zero mean and positive definite covariance, while the objective function penalizing squared input and state deviations was minimized. As in many MPC algorithms, LQG had also two weighting matrices for controller and set-point tracking concerns. Unlikely other MPC methods, LQG algorithm had infinite prediction horizon that ensured a powerful and robust stabilizing character.

In the following years, extensions to handle controlling outputs, off-set control and computing steady-state were handled (Kwakernaak&Sivan,1972). However constraint handling and state identification issues were not addressed in LQG theory. LQG became a standard approach in the industry for a wide range of applications with thousands of real-world applications and roughly 400 patents per year based on the Kalman filter (Goodwin, Graebe and Salgado, 2001). Despite that wide range of applications, LQG received a little attention in control theory. Richalet et al. (1976) and Garcia et al. cited the reasons of that little attention as :

- weakness in constraint handling
- failures in process nonlinearities
- lack of robustness in case of model uncertainties
- lack of unique performance criteria
- cultural reasons, reluctance of employees to new method.

It should also be noted that another key figure of MPC algorithm, controlling a system by solving a sequence of open-loop dynamic optimization problem has also been discussed since 1960s. Propoi (1963) described a moving horizon control theory and Lee and Markus (1967) stated the logic of moving horizon concept in control.

2.1.2. Model Predictive Heuristic Control (MPHC) and Identification & Command (IDCOM)

Despite all these academic studies, the gap between theory and practice was closed by two studies emerging form industry in the late seventies and started the MPC era.

In 1978, Richalet et al. summarized the first description of MPC control applications which was presented in 1976 IFAC Conference (Richalet et al., 1976). The approached was named as Model Predictive Heuristic Control (MPHC) and the solution software was referred as IDCOM, an acronym for Identification & Command.

Richalet et al. (1978) stated the main challenge as “with the availability of much powerful computers, should not the basic approaches to control system applications be considered?”. Indeed with more powerful computers with faster computation skills, fast access memory and higher storage capacities enhance the use of model and control history of process at each time step. The distinguishing features of IDCOM approach was summarized by Qin and Badgwell, 2003 as:

- impulse response model for the plant, linear in inputs or internal variables,
- quadratic performance objective over a finite prediction horizon,
- future plant output behavior specified by a reference trajectory,
- input and output constraints included in the formulation,
- optimal inputs computed using a heuristic iterative algorithm, interpreted as the dual of the identification.

Richalet et al. defined a model where inputs – output representation of the process. The process parameters were divided into sub categories. Inputs were categorized as manipulated variables (MV); inputs that were adjusted by the controller and disturbances; inputs that controller could not control. Due measuring capabilities of the system, disturbances were defined as measured disturbances (MD) and unmeasured disturbance (UD). The process outputs were referred as controlled variables (CV). The system related the inputs to influence the outputs directly.

MPHC algorithm was using an impulse model in which the model predicts the output at a given time depends on a linear combination of past input values. This model was obtained by evaluating the real plant data. The iterative nature of the control algorithm allows the constraints to be checked at each sampling time. Because the control law was not linear and could not be expressed as a transfer function, Richalet et al. (1978) referred as heuristic control, though it is called linear MPC today.

The MPHC algorithm drives the predicted output future trajectory as closely as possible to a reference trajectory, defined as a first order path from the current output value to the desired trajectory. By this way, controller provides a natural way to control the aggressiveness of the algorithm; increasing the time constants lead to a slower but more robust controller. Using impulse model for identification of the multivariable system was considered and the procedure was reported to save time in identification. It was suggested that, assuming linearity in the neighborhood of an operating point, the most appropriate model is the impulse response model

Rather than a fixed set point, IDCOM used a reference trajectory. The reference trajectory enhanced desired characteristics, like no overshoot or fixed time response. Robustness of the control system was also adjusted by reference trajectory.

Richalet et al. described the MPHC application to a fluid catalytic cracking unit (FCCU) main fractionator column, a power plant steam generator and a poly-vinyl chloride plant. Benefits from these three constraint cases were reported as $150,000/yr for fractionator column and $220,000/year for poly-vinyl chloride plant.

2.1.3. Dynamic Matrix Control (DMC)

An independent MPC technology was developed by engineers in Shell Oil in early seventies, with an initial application in 1973. However, the details of developed unconstrained multivariable control algorithm were not reported until 1979. The method was presented in the National AIChE meeting in 1979 and Joint Automatic Control Conference in 1980 by Cutler and Ramaker (Cutler and Ramaker, 1980). The distinguishing features of DMC approach was summarized by Qin and Badgwell, 2003 as:

- linear step response model for the plant, linear in inputs or internal variables,
- quadratic performance objective over a finite prediction horizon,

- future plant output behavior specified by trying to follow the setpoint as closely as possible,
- optimal inputs computed as the solution to a least-squares problem

DMC was very successful in overcoming the main problem of LQG control, because DMC represents a revolutionary contribution in communicating the needs of industry in a fashion that both industry and academia can understand. Garcia and Morshedi (1986) stated that fact as DMC “contained very transparent tuning parameters of physical meaning to the user”. This ease of use and effectiveness give the result as “Today there is probably not a single major oil company in the world where DMC is not employed in most new installations or reconstructs” (Morari and Lee, 1999).

Key features of DMC algorithm include use of a step response for calculation of the future errors of the system, which is the integral of impulse model used by IDCOM. Multiple outputs were handled by the superposition. Using the step response model, the predicted future output changes could be written as a linear combination of future output moves. The bound between these two was sustained via “Dynamic Matrix”. The quadratic objective function employed in DMC has two terms. One term represents the difference between the output and the reference trajectory and aim to adjust the set-point tracking capability. The other term represents the control move, penalizing the control effort to adjust the change in the manipulated variables to minimum. Tuning is carried out by manipulating these two terms, first one representing minimum error and the latter the robustness.

In DMC design, step response model was used instead of impulse model used in MPHC. Also quadratic performance objective function over a finite prediction horizon was used and future behavior of the plant was specified to follow the set point.

Cutler and Ramarker declared the results of the controller for a furnace temperature control. It was shown that the feed forward response of DMC algorithm was superior to that PID lead/lag compensator.

The main similarities between DMC and MPHC were summarized by Martin (1981) as both methods:

- utilized a non-minimal model presentation,

- considered predictive values of the controlled variable to find the future errors of the controlled process,
- made use of an internal method,
- updated the future predictions by using the actual measurements
- had a tuning parameter to dampen the control action.

2.1.4. Quadratic Dynamic Matrix Control (QDMC)

Beyond all advantages of DMC and MPHC, there were drawbacks in constraint handling of multivariable cases. In order to overcome those problems, Cutler addressed a quadratic program in DMC algorithm in a 1983 AIChE Conference and the algorithm was later explained in detail by Garcia and Morshedi (1986). Key figures of QDMC include:

- linear step response for the model,
- quadratic performance objective over a finite prediction horizon,
- future plant output behavior specified by trying to follow the set point as closely as possible subject to a move suppression term,
- optimal inputs computed as the solution to a quadratic program (Qin and Badgwell, 2003).

DMC quadratic objective function was rewritten in the form of a standard quadratic program. Future projected outputs were related with the input move vector through the dynamic matrix and by that way input and output constraints were collected into a matrix inequality involving the input move vector. The quadratic programming gradient vector, first derivative, was calculated at each sampling time, while quadratic programming Hessian matrix, second derivative, was calculated only once. The output constraints were reevaluated in the forms of input constraints using the system dynamic matrix.

Garica and Morshedi (1986) presented the results of QDMC on a pyrolysis furnace. The fuel gas pressures in three burners and bounds on temperature zones were presented as the constraints of the system. The test results were reported as successful for problems as large as twelve process inputs and twelve process outputs case. It was concluded that QDMC algorithm had proven particularly profitable in and on-line optimization environment.

2.1.5. IDCOM-M, HIECON, SMCA and SMOC

With the successful applications of DMC, MPHC and QDMC, the MPC strategy gained bigger interest and acceptance. The wider it was investigated, the more complex problems were acquainted. Especially the constraint handling problem and solving the objective function in one function were the main obstacles. Prett and Garcia (1988) commented on that problem: “The combination of multiple objectives into one objective function does not allow the designer to reflect the true performance requirements”. As a result the following studies were mainly focused on multi input – multi output (MIMO) case.

A modified version of IDCOM, as IDCOM-M was presented by Setpoint Inc, where the M denotes MIMO structure. Nearly at the same time, Adersa introduced its algorithm as hierarchical constraint control (HEICON). The controller was described by Grosdidier, Froisy and Hammann (1988) and main features were summarized as:

- linear impulse response of the model,
- controllability supervisor to screen ill-conditioned plant subsets,
- multi-objective function formulation; quadratic output objective followed by a quadratic input objective,
- controls a subset of future points in time for each output, called the coincide points, chosen from a reference trajectory,
- a single move is computed for each input,
- constraints can be hard or soft, with hard constraints ranked in order of priority (Qin and Bagdwell, 2003).

The IDCOM-M algorithm was different in the sense of using two separate objective functions, one for the outputs and one for the inputs. The desired output value was coming from a first order reference trajectory. Grosdidier et al. (1988), represented the capacity of the control for the FCCU problem, which was the case study of original IDCOM. The control problem was to control the flue gas composition, flue gas temperature and regenerator bad temperature by manipulating feed oil flow rate, recycle oil flow rate and air flow rate to the regenerator. The system was tested for three cases. First case showed the successful operation of multi input-multi output control. The second case showed the constant measured disturbance rejection capacity. The third case demonstrated the need for the controllability supervisor, where on manipulated variable failed, the controller was set to choose the optimum control strategy.

After introducing IDCOM-M, Setpoint Inc. represented Setpoint Multivariable Control Architecture (SMCA). SMCA offered an improved solution engine to solve a sequence of separate steady-state target optimizations. By this way a natural way to incorporate multiple control objectives and constraints was sustained.

By the end of 1980's Shell's research team in France introduced Shell Multivariable Optimizing Controller (SMOC). Marquis and Broustail (1998) stated the idea that the developed model was a bridge between state-space and MPC algorithms. The aim was to combine the successful constraint handling ability of MPC algorithm with the richer framework of state-space models. The model was testes on a hydrotreater unit with four reactor beds in series. The control aim was to control the reactor temperatures and the temperature variations between reactors at the desired reference value. Maximum temperature limitations were the constraints, while first reactor inlet temperature and quench flows between reactors were the manipulated variables. State-space model was shown to play a natural role to overcome the temperature dependence of reactors. Qin and Bagdwell (2003) summarized the key figures of SMOC algorithm as:

- State-space models were used so that the full range of linear dynamics could be represented,
- An explicit disturbance model described the effect of unmeasured disturbances; the constant output disturbance was simply a special case,
- A Kalman filter was used to estimate the plant states and unmeasured disturbances from output measurements,
- A distinction was introduced between controlled variables appearing in the control objective and feedback variables that were used for state estimation,

- Input and output constraints were enforced via a quadratic program formulation.

Beyond IDCOM-M, SMCA, HEICON and SMOC, several important algorithms were introduce in the late 1980's; including Profimatics' PCT algorithm and RMP algorithm by Honeywell.

2.1.6. DMC-plus and RMPCT

With the successful implementations of MPC algorithms, MPC vendors started to clear their position in the control market and tried strengthen their positions. Honeywell purchased Profimatics Inc and its algorithm PCT in 1995 and merged its RMPC algorithm to create RMPCT. In the same manner, Aspen Technology Inc purchased Setpoint Inc with its product SMCA and DMC Corporation with product DMC to create DMC-plus. The key figures of these combined technologies were summarized by Qin and Bagdwell (2003) as:

- windows-based graphical user interfaces,
- multiple optimization levels to address prioritized control objectives,
- additional flexibility in the steady-state target optimization, including quadratic programming and economic objectives,
- direct consideration of model uncertainty (robust control),
- improved identification technology based on prediction error method and sub-space identification methods.

2.2 Other MPC Algorithms and MPC Applications to Chemical Reactor Control

After the successful applications which are referred as first and second generations MPC in Figure 2.1, a growing number of researches became available in the academia. Since MPC is an open code with main principles; use of an explicit model, optimization at each time step and use of future time horizon, variations of these concepts lead to many researches. Variations in optimization techniques, investigation on robustness, tuning techniques, adaptation with other techniques like neural networks or fuzzy control have been studied by many researchers since then.

Rouhani and Mehra (1982) developed mathematical issues and fundamental components of control structure for their model and referred as Model Algorithmic Control (MAC) instead of MPC. Rouhani and Mehra (1982) suggested that an off-line identification of the plant is adequate, since online identification brought burden to computation. MAC algorithm used an impulse response. Differing form DMC, control horizon was not considered as a tuning parameter in MAC algorithm and was taken equal to the prediction horizon. The single input – single output case was examined in detail and for both deterministic and stochastic environment stability and robustness was evaluated.

It was shown by Marchetti et al. (1983) that under certain circumstances, MAC algorithm can be defined to reflect a dead-beat type controller. Marchetti et al. (1983) also compared a single input – single output controller and a discrete PID controller for three representative process models and for an experimental continuous stirred tank heater. It was concluded that the predictive controller was quite effective, but they stated that a single input – single output controller did not utilize full capabilities of the predictive controller as in multivariable cases. Also a significant reduction in the dimensions of dynamic matrix was tested and shown not to significantly degrade the control system performance.

Garcia and Prett (1986) summarized the current situation in model predictive controllers where all mathematical backgrounds of linear, unconstrained, constrained model predictive controllers are given and also the application of DMC on a heavy oil fractionator is studied as a case study.

Clarke et al. (1987a) proposed a new control algorithm called Generalized Predictive Controller (GPC). The aim was to obtain a control rule for handling larger range of control problems for larger range of plants. The method was claimed to be applicable to non-minimum phase or poorly identified plants with unknown order or dead time and to open loop unstable systems (to which DMC, MPHC and similar algorithms were not applicable without certain adjustments). In GPC, the process model was developed in discrete time and a disturbance term was included. These types of models are called "controlled auto regressive and moving average" (CARMA) models. More detailed discussions on extensions of GPC were discussed in the following paper by Clarke et al. (1987b) In order to overcome the problem of models of disturbances (such as changes in material quantity or quality), the CARMA model was divided by a differencing operator and "controlled auto regressive integrated moving average" (CARIMA) model was obtained (Camacho and Bordons, 1999). The major drawback of GPC was stated by Morari and Lee (1999) as "not being suitable for multivariable constrained systems, more commonly encountered in the oil and chemical industries".

Garcia et al. (1989) showed that all of the existing MPC algorithms, including MPHC, DMC and internal model control (IMC) and made their comparisons. After this study, the generic term Model Predictive Control was used for this class of algorithm. They suggested that there is a significant advantage of MPC in terms of the overall operating objectives of the process industries. Applications of MPC were also investigated for nonlinear systems and main attractions were identified.

Riggs and Rhinehart (1990) compared nonlinear internal model control (IMC) and generic model control (GMC) on a single input – single output (SISO) exothermic continuous stirred tank reactor (CSTR) and SISO heat exchanger. It was concluded that both methods were relatively intensive to process/model mismatch for nonlinear systems and have relatively wide tuning bands.

Sistu and Bequette et al. (1992) studied a comparison of globally linearizing control (GLC), a differential geometry based control, and nonlinear predictive control (NLPC), an optimization based technique, for temperature control of an exothermic continuous stirred tank reactor (CSTR). GLC linearize the output/input or the state/input closed loop nonlinear system. This technique was only used on minimum phase systems, in which the inverse dynamics were stable. All state variables assumed to be measured for GLC. If there were unmeasured state variables, estimation techniques must be used. The results were obtained for considering perfect model, with measured and unmeasured disturbances, an uncertain model, and finally constraints on manipulated variable. For an unconstrained case, GLC gave same performance to NLMPC. However, NLMPC gave beter performance than GLC considering constraints on manipulated variable.

Lee et al. (1994) proposed a new control scheme, which consisted of an Adaptive Model Predictive Control (AMPC) and state feedback control, for unstable nonlinear processes. Then, the final control inputs were the summation of feedback outputs and the control actions of the AMPC. The control law of AMPC was similar to that of Dynamic Matrix Control (DMC) but the output prediction was obtained by ARMAmodels, which is very useful for model parameter identification, in AMPC. The advantages of this proposed method were easy implementation to unstable nonlinear processes with robustness and simplicity of design. The performance of AMPC was tested by ajacketed continuous stirred tank reactor (CSTR) and two jacketed CSTRs in series with a seperator and compared with Generalized Predictive Control (GPC) and Adaptive Generalized Predictive Control (AGPC). The results showed that AGPC gave good performance for good set-point tarcking, in contrast GPC failed to overcome the effect of process change, and AMPC showed better stable control performance than AGPC.

Santos et al. (2001) implemented a nonlinear model predictive control (NMPC) algorithm in a continuous stirred tank reactor (CSTR). The objective was to control the liquid level and temperature in the pilot plant where an irreversible exothermic chemical reactions simulated experimentally by steam injection. A first principle model was used to observe the dynamic behavior of the plant and that dynamic behavior was compared with the experimental data. The nonlinear MPC algorithm was shown be very useful for processes operating at or near singular points that cannot be captured by linear controllers and where higher order information is needed. Nonlinear MPC was using a nonlinear dynamic model to predict the control steps effects on the controlled variables by deriving the output variables to the desired steady state setpoints, based on environmental, economic, safety and product quality considerations. The study showed that the model showed a very nonlinear behavior and was validate with the experimental data. Although it was appeared to have quite successful comparison between the experimental and the plant data, several sources of unmeasured disturbances as well as a significant degree of plant/model mismatch within the system. Despite these challenges, successful set point tracking and disturbance rejection was observed.

Prasad et al. (2002) applied a multivariable multi-rate nonlinear MPC. The model was tested for styrene polymerization in a continuous stirred tank reactor. The control objective was to control of polymer properties such as number average molecular weights and polydispersity. The NMPC algorithm included a multi-rate Extended Kalman Filter (EKF) in order to handle state variable and parameter estimation. The multi-rate EKF was used for the design of the augmented disturbance model as estimator. Plant-model structural mismatch, parameter uncertainty and disturbances were considered for control simulations in open loop unsteady state CSTR. The results for the proposed control algorithm were shown to have superior performance compared to linear multi-rate and nonlinear single rate MPC algorithms.

Afonso et al. (1996) investigated the performance of a receding horizon model predictive control applied to a real plant in order to show the applicability of model predictive controllers to real life beyond simulations. Continuous stirred tank reactor (CSTR) was chosen as the experimental case, where an industrial pseudo zero order exothermic chemical reaction was simulated in order to control temperature and level of the reactor. By making MPC algorithm formulation, the manipulated variables were calculated so as to minimize an objective function considered desired trajectories over the horizon. The rate of heat generated by reaction was calculated and converted into an equivalent steam flow rate. The performance of receding horizon model predictive control applied in a CSTR was compared with PI controller. A significant controller performance was said to be achieved with MPC when compared with the previously existing PI controller, operating in steady state or dynamically, despite both MPC and PI strategies showed the similar performance for level control.

Park and Rhee (2001) studied a linear matrix inequality (LMI)-based robust model predictive control. The controller was applied to control the polymerization of methyl methacrylate in a continuous stirred tank reactor. The polytopic model was constructed to predict the responses to various control input sequences by using Jacobians of uncertain nonlinear model at several operating points. The controller was designed to minimize an upper bound objective function subject to constraints on the control input and plant output. The controller performance was checked for two cases; SISO and MIMO. In the SISO system, the manipulated variable was the jacket inlet temperature and the controlled variable was the monomer conversion. In MIMO system, the manipulated variables were the jacket inlet temperature and the feed flow rate, the controlled variables were the monomer conversion and the weight average molecular weight. According to the simulation results, despite the model uncertainty, the LMI-based robust model predictive controller performed quite satisfactorily for the property of continuous polymerization reactor and the robust stability was guaranteed.

Biagiola and Figueroa (2004) proposed an application of state estimation based nonlinear model predictive controller to an unstable nonlinear process. The nonlinear process was chosen to be a jacketed exothermic reactor and control aim was to control the temperature of the reactor at a desired level. A state-space formulation was proposed to achieve the control objective. To update the optimization involved in nonlinear MPC strategy, state estimation based on the measured output was proposed. The computer simulations were developed for the performance of the nonlinear observer and the control strategy.

Wu (2001) studied robust model predictive controller for a class of uncertain linear systems with structured time varying uncertainties, linear fractional transformation perturbations. The controller was designed to characterize as an optimization problem of the worst-case objective function over infinite moving horizon. An adequate state-feedback synthesis condition was developed and formulated as LMI optimization. Then, the control action could be calculated on-line. The stability of controller was decided by the feasibility of the optimization problem. The performance of the robust MPC technique was implemented to an industrial CSTR with a first order, irreversible exothermic reaction with explicit input and output constraints for set point tracking without disturbance and disturbance rejection. According to simulation results, it was concluded that robust MPC technique was capable of incorporating model mismatch and constraints.

Al-Ghazzawi et al. (2001) offered a tuning strategy based on the linear approximation between the closed-loop predicted output and the model predictive control tuning parameters. Linear model predictive controllers (LMPC) based on finite impulse response (FIR) models were developed. Al-Ghazzawi developed analytical expressions for the sensitivity of the closed-loop response of MPC with respect to output and input weights of the objective function. Both of the control and prediction horizon were kept constant predetermined values by depending on conventional tuning guidelines. The controller strategy performance was illustrated by using a linear model for a three product distillation column and a non-linear model for a CSTR. In CSTR, where an exothermic catalytic reaction was taking place, a linearized model was developed and converted to FIR to use it for MPC algorithm. The set point tracking, disturbance rejection and effect of modeling errors were considered, the performance of proposed method gave good results. There is also a comparison of the proposed on-line tuning method with an existing off-line tuning method. The off-line method had the control performance better than the proposed method. In addition to that off-line method expressed a considerably high sluggish response in distillation column example and unstable response in the CSTR example.

Nagrath et al. (2002) developed a state estimation based model predictive control approach that had the same general philosophy with cascade control, which was examined to be commonly used in the operations of chemical processes to reject disturbances that had a rapid effect on the measured state. The designed MPC was presented to be superior to cascade control in the additional advantage of constraint handling capacity. The proposed controller was checked via an exothermic jacketed continuous stirred tank reactor, where the jacket temperature was used as a secondary measurement in order to infer disturbances in the jacket feed temperature and reactor feed flow rate. The state estimation was sustained by using a Kalman filter while a quadratic programming (QP)-based optimization for the predictive controller explicitly handled the manipulated variable constraints. The cascade strategy based model predictive controller scheme was compared to classical cascade control, and it can be shown that MPC-based cascade method performed better than it in the presence of constraints on jacket flow rate.

A nonlinear model predictive control was presented by Biegler et al. (2002) based on a Wiener piecewise linear model. The LHN approach was used for Wiener model identification since it was to be straightforward and guarantee an accuracy of the static nonlinearity. After identifying the linear block by using a correlation technique, the intermediate signal was generated from the input signal and finally the static non-linearity was estimated. A good representation of the inverse of the nonlinearity was necessary to implement NMPC algorithm. In order to identify it, direct identification, which was the identification of the nonlinear element of the model but switching inputs and outputs, was used. This proposed technique was illustrated by a SISO CSTR and a MIMO polymerization reactor and the response of NMPC and LMPC are compared. The results showed that the LMPC step response to a lower set point was slower but LMPC was faster for an upper step input.

Hidalgo and Brosilow (1990) proposed a combination of a nonlinear model predictive controller and Coordinated Control. The combination yield to an effective control for reactors operating around an unstable operating point. The controller was checked for the continuous stirred tank reactor, in which free radical solution polymerization styrene monomer reaction took place. By manipulating the reactant styrene rate and the coolant flow rate, the product concentration was being controlled. Hidalgo and Brosilow (1990) reported successful set point tracking for steady state, although significant modeling errors were present.

2.3 Future of MPC Algorithms

Beyond wide spread applications of Model Predictive Controller algorithms especially in the refinery and petrochemical industry, there is still an important area of possible practice area. Qin and Bagdwell (2003) summarized a composite view of MPC technology's future. In this study, the main focus points for future MPC algorithms were summarized as basic controller formulation, adaptive MPC, Robust MPC and nonlinear MPC.

As the systems to be controlled become more and more complex, it is not easy and meaningful to express all control objectives in single objective function. Qin and Bagdwell (2003) suggested that future MPC algorithms deal with multiple objective functions. With increasing computational power, prediction horizons would tend to be infinite rather than a proportion of a model horizon. Input parameterization using basis functions may become widespread and infinite control horizons with moves computed at each control interval would be possible.

Although there is a remarkable need in the industry for adaptive control systems, the difficulty of adaptive control in the real world prevents those applications. As stated above, Generalized Predictive Controller (GPC) was the first adaptive MPC algorithm and was not found to be successful. Qin and Bagdwell (2003) forecasted that lack of adaptive control would not change in the near future. Adaptive PID controllers were assumed to be an adequate solution for the industries' needs.

MPC control algorithms rely solely on evaluating model mismatch and robustness. Robust control schemes would decrease the effort for tuning and testing in the industry. There are several successful robust MPC applications reported like, Kassmann et al. (2000), Kothare et al. (1996) and Scokaert and Mayne (1998). Robust designs would be more available in the future market.

Although MPC strategies are widely used in the petrochemical and refinery industries, more nonlinear the systems become, the less MPC finds place. As can be seen from Figure 2.2, there is a large untouched area of applications for MPC algorithms. The main reason of this open area is the increasing nonlinearity. Qin and Bagdwell suggested that next generation MPC technology would allow nonlinear models to be developed by combining process knowledge and operating data. Process test signals would be designed automatically so as to explore important regions of the operating space where the model is inadequate to control.

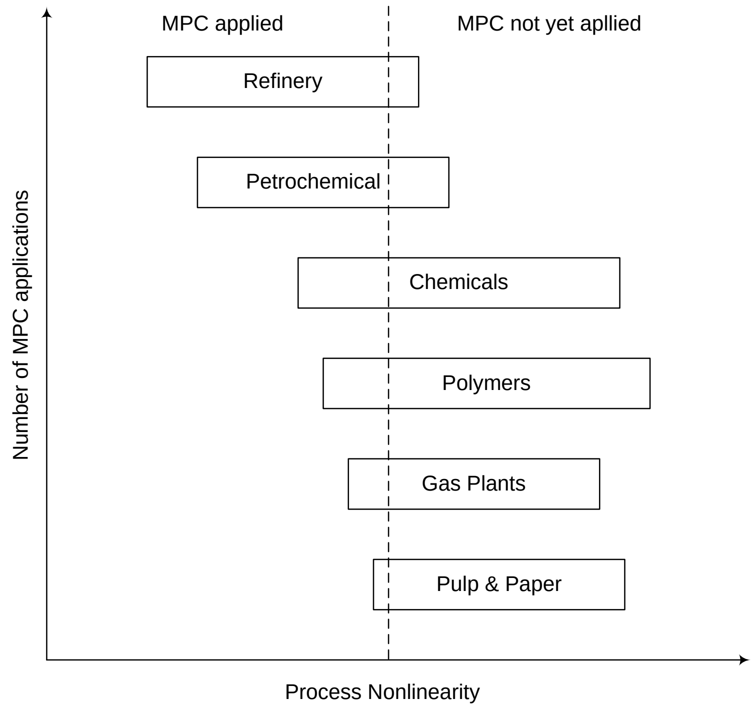


Figure 2.2 : Distribution of MPC applications vs the degree of process nonlinearity, (Qin and Badgwell, 2000)

3. MODEL PREDICTIVE CONTROL (MPC)

3.1 MPC Strategy

Camacho and Bordons (1999) offered an analogy for the sake of understanding MPC strategy. The strategy is very similar to the control strategy used in driving a car as in Figure 3.1. The driver knows the desired reference trajectory for a finite control horizon, and by taking into account the car characteristics (mental model of the car) decides which control actions (accelerator, brakes and steering) to take in order to follow the desired trajectory. Only the first control actions are taken at each instant, and the procedure is repeated for the next control decisions in a receding horizon fashion. With control schemes, driver can only use the car with a mirror and can take action after a deviation occurs.

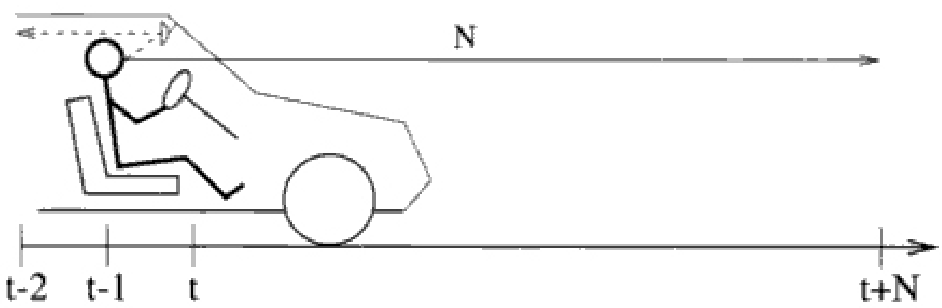


Figure 3.1: MPC analogy with car driving (Camacho and Bordons, 1999)

MPC strategy can be better understood by the use of Figure 3.2. The main strategy of MPC controllers can be summarized in three steps (Camacho and Bordons, 1999). At an arbitrary sampling instant k, the future values of the system for a period of P discrete time steps (prediction horizon) (y(t+k) for k=1…P) are predicted at each instant by making use of the system's model available with past input applied and future inputs to be applied to the process. Past inputs (u(n-1), u(n-2)…,u(n-C+1)) are represented in solid lines in Figure 3.2, where dashed lines represent the future inputs (u(n), u(n+1),…,u(n+C)).In the second step, the set of future signals is calculated by optimizing a determined criterion in order to keep the process as close as possible to the reference trajectory, (r) in Figure 3.2. Only the first element of the future input is applied to the process since a new measurement of the output can be present in the next sampling instant. The procedure is repeated at each sampling instant with new measurements, which is called the receding strategy.

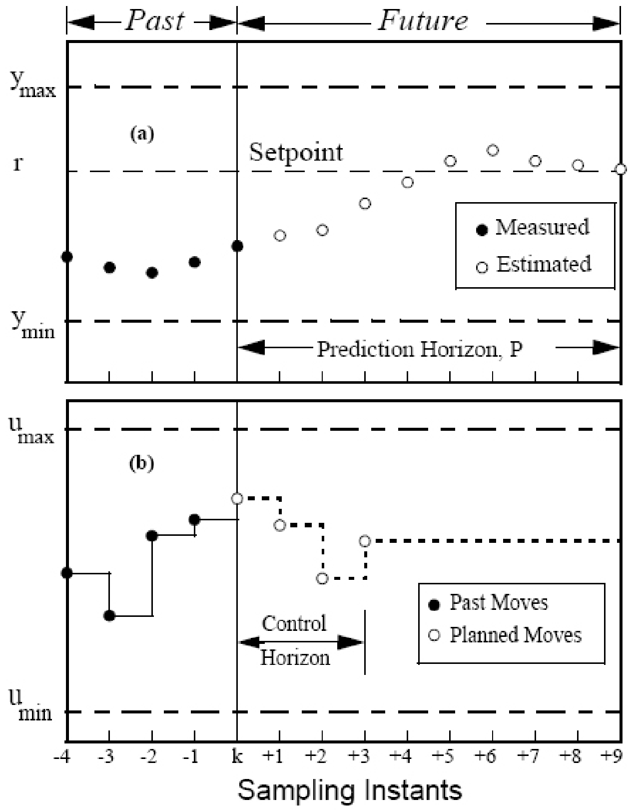


Figure 3.2: MPC Strategy (Bemporad et al.,2006)

In order to implement MPC strategy, the basic structure in Figure 3.3 is used.

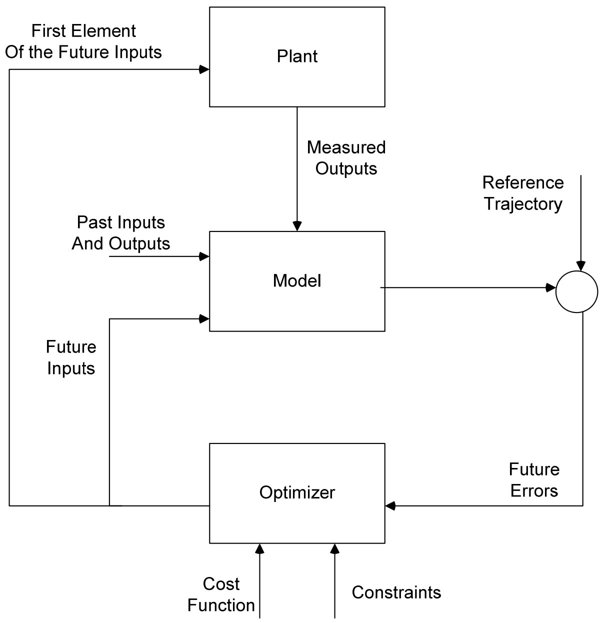


Figure 3.3: Basic structure of MPC (Camacho and Bordons, 1999).

As shown in Figure 3.3, a model uses past inputs and outputs of the system with the future inputs and predicts the plant's future state. The predicted outputs are than compared with the reference trajectory and future errors are calculated. These future errors are optimized in the presence of constraints with objective function and optimizer sends the set of future control actions to the model. While doing so, only the first element of the future inputs is sent to plant to realize and the response of the plant is used to correct the model at each sampling period.

3.2 MPC Prediction Model

The model is the corner-stone of MPC; a complete design should include the necessary mechanisms for obtaining the best possible model (Camacho and Bordons, 1999). The most common prediction model used in MPC design is the step response model, or namely discrete convolution model. The major advantage of the step response modeling is that, there is only need for input – output information of the process without concerning the model's restrictions. Figure 3.4 represents an open loop step response of a linear process.

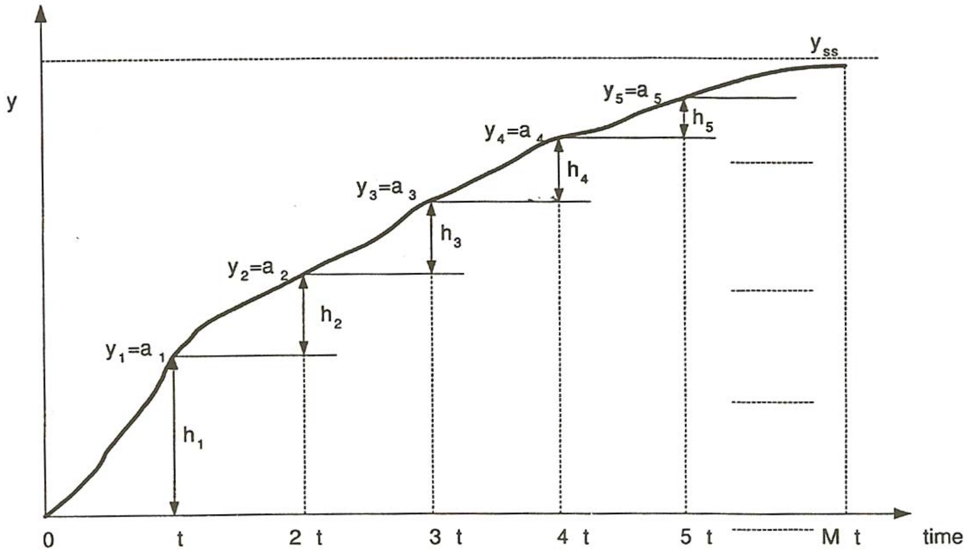


Figure 3.4: Open loop step response of a linear process (Seborg et al., 1989).

Where 'u' represents inputs and 'y' is used to define outputs. The step response, obtained by giving a 1-2 % magnitude step change to the process, would tend to stabilize and the h_i values tend to be zero. In other words, the subsequent a_i values tend to be equal.

$$\lim_{t \to \infty} a_i = a_{i-1} \quad \text{and} \quad \lim_{t \to \infty} h_i = 0 \tag{3.1}$$

The 'a' values represent the step response coefficient and 'h' values represent impulse response coefficients. For an open loop step response representation, the step response coefficients are the summation of all impulse response coefficients.

$$a_i = \sum_{j=1}^{i} h_j \tag{3.2}$$

The time required to reach the 99 % of the final value of the system is defined as the Model Horizon (M). Since M is an interval term, the time required for model horizon can be obtained simply multiplying M with sampling time.

Using open loop system response, for model horizon M input changes to predict the system's output, the discrete convolution method is written as:

$$\hat{y}_1 = y_0 + a_1 \Delta u_0 \qquad (3.3)$$

$$\hat{y}_2 = y_0 + a_2 \Delta u_0$$

.

.

$$\hat{y}_M = y_0 + a_M \Delta u_0$$

Where the superscript ^ denotes the predicted values. Also it should be noted that $\Delta u = u_i - u_{i-1}$. If this representation is modified to predict the system's output to every possible input change that can be introduced at each instant the resulting equation becomes

$$\hat{y}_{n+1} = y_0 + \sum_{i=1}^{M} h_i u_{n+1-i} \qquad (3.4)$$

In order to incorporate the model errors and disturbances:

$$y_n - \hat{y}_n = y^*_{n+1} - \hat{y}_{n+1} \qquad (3.5)$$

can be written. The suffix * is used to represent the real output value of the process. Equation 3.5 states that the difference between the predicted and the measured value is assumed to be constant for the next sampling time. This error value can be used to treat the model misprediction.

Substituting Equation 3.5 into Equation 3.4 gives:

$$y^*_{n+1} = y_n + \sum_{i=1}^{M} h_i u_{n+1-i} \qquad (3.7)$$

When it is assumed that the same amount of error takes place in the discrete time of the model during prediction horizon, Equation 3.6 can be expanded for the prediction horizon, P as:

$$y^*_{n+j} = y^*_{n+j-1} + \sum_{i=1}^{M} h_i u_{n+j-1} \quad \text{For } j=1,2,\ldots,P \qquad (3.8)$$

3.3 MIMO Representation of the Step Response Model

The single input – single output system defined in the previous section is not applicable for most of the models. Because of that reason MIMO extension of step response model for 2x2 system is developed using the superposition principles as Equation (3.7).

$$y^{*}_{1,n+j} = y^{*}_{1,n+j-1} + \sum_{i=1}^{M} h_{11,i} u_{1,n+j-1} + \sum_{i=1}^{M} h_{12,i} u_{2,n+j-1} \qquad (3.9)$$

$$y^{*}_{2,n+j} = y^{*}_{2,n+j-1} + \sum_{i=1}^{M} h_{12,i} u_{1,n+j-1} + \sum_{i=1}^{M} h_{22,i} u_{2,n+j-1} \qquad \text{For j=1,2…,P}$$

3.4 Objective Function

MPC algorithm follows a reference trajectory by the future outputs on the prediction horizon and penalizes the control effort on the control horizon. General objective function of the MPC can be written as:

$$\min_{\Delta u(n)\ldots\Delta u(n+C-1)} \sum_{i=1}^{P} \left\| \hat{y}(n+i) - r(n+i) \right\|^{2} w_1 + \sum_{j=1}^{C} \left\| \Delta u(n+i-1) \right\|^{2} w_2 \qquad (3.10)$$

In the optimization problem given in Equation 3.10, the first term is used to minimize the error resulting from the difference between predicted outputs and reference trajectory, 'r' during prediction horizon, P. The second term is the difference of control actions taken at each time step during control horizon, C. Equation 3.10 can be expressed literally as Equation 3.11:

$$\min_{\Delta u(n)\ldots\Delta u(n+C-1)} \sum_{i=1}^{P} \left\| setpo\,\mathrm{int} - prediction \right\|^{2} w_1 + \sum_{j=1}^{C} \left\| inputcahnges \right\|^{2} w_2 \qquad (3.11)$$

Weighting matrices w_1 and w_2 are positive definite matrices, with the magnitude of (CxC) and (PxP) respectively. These matrices are usually diagonal, real symmetric positive definite weighting matrices, and λ_1 and λ_2 represents the diagonal elements of the matrices. Through these matrices the closed loop behavior can be altered, therefore they are used as tuning parameters.

In tuning, rather than assigning values independently, a ratio λ is assigned; where $f=\lambda_1/\lambda_2$. The literature tends to keep λ_2 constant as 1 and change λ_1 as tuning parameter. Regarding to the choice of giving weight to penalizing the control effort or set point tracking capacity, the value of f would be altered.

3.5 Design of the Controller

MPC algorithm can be designed with step response model of a MIMO system. To do so, predicted values must be subtracted from corresponding set point (r) to give:

$$\begin{bmatrix} r_1 - y_{1,n+1} \\ r_1 - y_{1,n+2} \\ . \\ . \\ r_1 - y_{1,n+P} \\ r_2 - y_{2,n+1} \\ r_2 - y_{2,n+2} \\ . \\ . \\ r_2 - y_{2,n+P} \end{bmatrix} = -\begin{bmatrix} A_{11} A_{12} \\ A_{21} A_{22} \end{bmatrix} \begin{bmatrix} \Delta u_{1,n} \\ \Delta u_{1,n+1} \\ . \\ . \\ \Delta u_{1,n+C-1} \\ \Delta u_{2,n} \\ \Delta u_{2,n+1} \\ . \\ . \\ \Delta u_{2,n+C-1} \end{bmatrix} + \begin{bmatrix} r_1 - y_{1,n} + P_{1,1} \\ r_1 - y_{1,n} + P_{1,2} \\ . \\ . \\ r_1 - y_{1,n} + P_{1,P} \\ r_2 - y_{2,n} + P_{2,1} \\ r_2 - y_{2,n} + P_{2,2} \\ . \\ . \\ r_2 - y_{2,n} + P_{2,P} \end{bmatrix} \qquad (3.9)$$

Where first row of A matrix indicates the first manipulated input’s effect on the first and second controlled outputs, second row indicates the second manipulated input’s effect on the first and second controlled outputs.

Equation (3.9) can be simplified as:

$$\hat{E} = -A\Delta u + \hat{E}' \tag{3.10}$$

There are two predicted error vectors where E' is the open loop prediction error of the process depicting the error that would have been made by the system over prediction horizon if no future control actions were taken. E is the prediction error of future and current errors.

The future control effort can be described as:

$$\Delta u^T w_2 \Delta u \tag{3.11}$$

The quadratic objective function can be rewritten as:

$$\Delta u = (A^T w_1 A + w_2)^{-1} A^T w_1 \hat{E}' = K_{MPC} \hat{E}' \tag{3.12}$$

where K_{MPC} is a constant.

3.6. Singular Value Decomposition

Singular Value Decomposition Method is used to observe the interaction between inputs and outputs. "SVD provides quantitative information about sensor placement, physical controllability, controller pairing and also can be used directly as a decoupling control strategy" (Moore, 1986).

In the Singular Value Decomposition method, the steady state matrix is written as:

$$G = U \Sigma V^T \tag{3.13}$$

where U is left singular vector, V is the right singular vector and Σ is called the singular values.

After forming G, the largest vector element of column U is paired with the largest vector element of V. The Condition Number (CN) is defined as the ratio of the largest and the smallest nonzero singular values. The larger the condition number, the more poor conditioning increased.

$$CN = \frac{\sigma_1}{\sigma_2} \tag{3.14}$$

4. CASE STUDY: PRODUCTION OF PROPYLENE GLYCOL

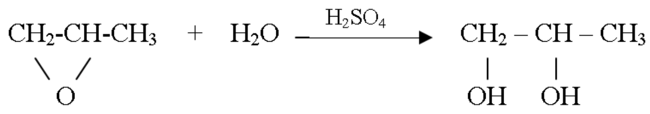
Performance of model predictive controller is examined in the production of propylene glycol from hydrolysis of propylene oxide in a continuous stirred tank reactor.

Propylene glycol, known also as 1,2-propanediol is a tasteless, odorless and colorless chemical. Its main uses are in (The Innovation Group Report, 2002):

- Unsaturated polyester resins (27%)
- Functional fluids; antifreeze, de-icing, heat transfer (20 %)
- Food, drug and cosmetic uses (20 %)
- Liquid detergents (17 %)
- Paints and coatings (5 %)
- Tobacco humectant (2 %)
- Miscellaneous (9 %)

The demand of propylene glycol in USA market shows a constant growth with 387,000 tones in 1999, 387,000 tones in 2000 and projection of 427,700 tones. The annual demand increase is forecasted as 2.0 %. Propylene glycol makes up about 25 % of the major derivatives of propylene oxide. The commercial price is in the range of $ 1.4 to 1.5 in 2004. Especially increasing demand in cosmetics in their emollient bases for personal care products such as antiperspirants and deodorants, suntan lotions and use as enzyme stabilizer in liquid detergent industry satisfies a solid market demand on the product.

Propylene glycol is produced by the hydrolysis of propylene oxide in the presence of sulfuric acid as catalyst:



(4.1)

In the CSTR, propylene oxide feed is in a mixture with methanol and reacts with excess water in an exothermic reaction. Due to the heat generation from exothermic reaction, temperature of the reactor is adapted by using a cooling coil with water as coolant.

The MPC algorithm is designed to control the product concentration and temperature inside the reactor. Model of the reactor and control strategy will be presented below.

Model of the Chemical Reactor

The model of the CSTR for propylene glycol production is developed from material and energy balances. Before deriving balance equations, assumptions below are made:

- Volume of the reactor is assumed to be constant,
- The densities of all components are assumed to be constant,
- The heat capacities of all components are assumed to be constant,
- A quasi steady state is assumed for energy balance on heat exchanger and accumulation term is neglected.
- Perfect mixing is assumed. Temperature of the reactor and concentration of product are assumed to be the same with exit flows temperature and concentration.

The set-up of CSTR is shown in Figure 4.1. For the sake of clarity, subscripts A for propylene oxide, B for water, M for methanol, CW for cooling water and C for propylene glycol are used. F is used for flow rates and C represents used for concentrations.

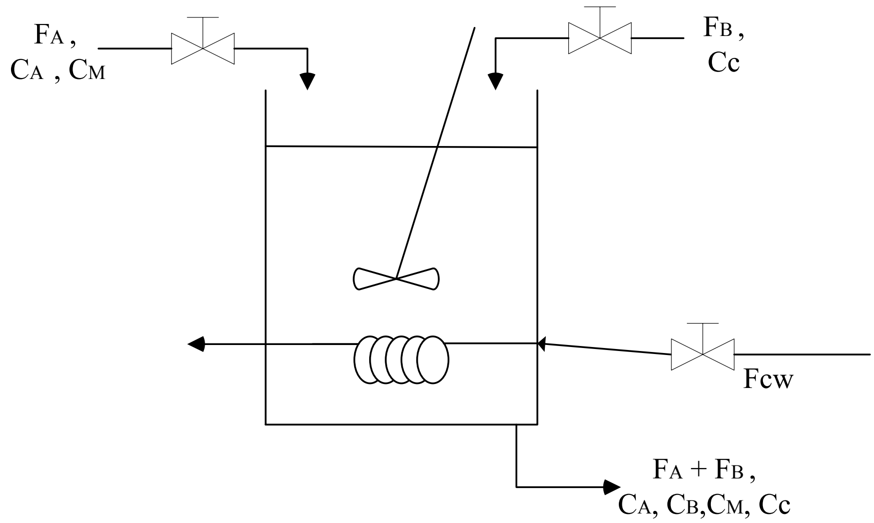


Figure 4.1 : Set-up of CSTR of propylene glycol production.

As noted before, propylene oxide and water react exothermally. Since the reaction occurs in the excess water, reaction is limited by propylene glycol with the reaction rate equation given in 4.2.

$$r_A = -k_0 C_A \exp(\frac{-E}{RT}) \tag{4.2}$$

Overall mass balance over the reactor for constant volume can be written as

$$F_{exit} = F_A + F_B \tag{4.3}$$

Mass balances of components in the reactor are

Propylene oxide balance:

$$\frac{dC_A}{dt} = (\frac{F_A}{V})C_{Ai} - (\frac{F_A + F_B}{V})C_A - k_0 \exp(\frac{-E}{RT})C_A \tag{4.4}$$

Water balance:

$$\frac{dC_B}{dt} = (\frac{F_B}{V})C_{Bi} - (\frac{F_A + F_B}{V})C_B - k_0 \exp(\frac{-E}{RT})C_A \tag{4.5}$$

Methanol balance:

$$\frac{dC_M}{dt} = (\frac{F_A}{V})C_{Mi} - (\frac{F_A + F_B}{V})C_M \tag{4.6}$$

Propylene glycol balance:

$$\frac{dC_C}{dt} = -(\frac{F_A + F_B}{V})C_C + k_0 \exp(\frac{-E}{RT})C_A \tag{4.7}$$

The energy balance around the reactor is written as

$$\begin{aligned}[V(C_A Cp_A + C_B Cp_B + C_M Cp_M + C_C Cp_C]\frac{dT}{dt} &= (F_A C_{Ai} Cp_A T_i) + \\ (F_B C_{Bi} Cp_B T_i) - (F_A + F_B)(C_A Cp_A &+ C_B Cp_B + C_C Cp_C + C_M Cp_M)T \\ + (\Delta H_{rxn} k_0 \exp(\frac{-E}{RT})C_A V) + Q\end{aligned} \tag{4.8}$$

Fogler (1999) defines the energy balance equation on heat exchanger as:

$$m_c Cp_{cw} T_{a1} - m_c Cp_{cw} T_{a2} - \frac{UA(T_{a1} - T_{a2})}{\ln[(T - T_{a1})/(T - T_{a2})]} = 0 \tag{4.9}$$

where T_{a1} and T_{a2} are ambient temperatures for inlet and outlet coolant temperatures of the heat exchanger, respectively.

$$m_c = \frac{F_{cw}\rho_w}{MW} \tag{4.10}$$

Simplifying equation (4.9),

$$Q = m_c Cp_{cw}(T_{a1} - T_{a2}) = \frac{UA(T_{a1} - T_{a2})}{\ln\left[(T - T_{a1})/(T - T_{a2})\right]} \qquad (4.11)$$

Solving equation (4.11) for outlet coolant temperature of the heat exchanger,

$$T_{a2} = T - (T - T_{a1})\exp(\frac{-UA}{m_c Cp_{cw}}) \qquad (4.12)$$

Using equations (4.11) and (4.12), equation (4.13) is obtained by solving for heat transfer rate, Q,

$$Q = m_c Cp_{cw}\left\{(T_{a1} - T)\left[1 - \exp(\frac{-UA}{m_c Cp_{cw}})\right]\right\} \qquad (4.13)$$

Equation (4.13) is substituted into the original energy balance equation (4.8) as,

$$\left[V(C_A Cp_A + C_B Cp_B + C_M Cp_M + C_C Cp_C\right]\frac{dT}{dt} = (F_A C_{Ai} Cp_A T_i) \qquad (4.14)$$

$$(F_B C_{Bi} Cp_B T_i) - (F_A + F_B)(C_A Cp_A + C_B Cp_B + C_C Cp_C + C_M Cp_M)T$$

$$+ (\Delta H_{rxn} k_0 \exp(\frac{-E}{RT})C_A V) + m_c Cp_{cw}\left\{(T_{a1} - T)\left[1 - \exp(\frac{-UA}{m_c Cp_{cw}})\right]\right\}$$

Using equations (4.4), (4.5), (4.6) and (4.7) for mass balance and (4.14) for energy balance the CSTR model is developed. The numerical values of constants are obtained from Fogler (1999) and Perry (1980). All numerical values are summarized in Table 4.1.

Table 4.1: Numerical values of CSTR design equations

Parameter	Definition	Value
F_A	Flow rate of propylene oxide and methanol mixture	0.733 lt/sec
F_B	Flow rate of water	1.833 lt/sec
F_{CW}	Flow rate of coolant, water	1.833 lt/sec
C_{Ai}	Initial concentration of propylene oxide entering the reactor	7.39 mol/lt
C_{Bi}	Initial concentration of water entering the reactor	55.17 mol/lt
C_{Mi}	Initial concentration of methanol entering the reactor	12.35 mol/lt
C_{Ci}	Initial concentration of propylene glycol the reactor	0.0 mol/lt
V	Volume of the reactor	1136 lt
T_i	Initial temperature of feed streams	297 K
T_{a1}	Initial temperature of coolant	293 K
k_0	Reaction rate constant	$4.711*10^9$ sec^{-1}
E	Activation energy	18000 cal/mol
R	The gas constant	1.9872 cal/mol-K
Cp_A	Heat capacity of propylene oxide	146.54 J / mol-K
Cp_B	Heat capacity of water (used also for coolant)	75.362 J / mol-K
Cp_C	Heat capacity of propylene glycol	192.59 J / mol-K

Table 4.1: Numerical values of CSTR design equations (cont'd).

Cp_M	Heat capacity of methanol	81.64 J / mol-K
ΔH_{rxn}	Heat of reaction	84667 J/mol
ρ_{CW}	Density of coolant	1000 kg/m^3
MW	Molecular weight of coolant	18.01 gr/mol
UA	Heat transfer coefficient * Heat transfer area	28.20 J / sec-K

Using equations (4.4), (4.5), (4.6) and (4.7) for mass balance and (4.14) for energy balance, the differential equations were solved with Matlab and steady state values response and steady state concentrations for four chemicals and reactor temperature were obtained and tabulated in Table 4.2.

Table 4.2: Steady state values for concentrations and temperatures

Parameter	Definition	Value
C_{Ass}	Steady state concentration of propylene oxide	0.01037 mol/lt
C_{Bss}	Steady state concentration of water	37.31 mol/lt
C_{Mss}	Steady state concentration of methanol	3.5279 mol/lt
C_{Css}	Steady state concentration of propylene glycol	2.1006 mol/lt
T_{ss}	Steady state temperature of the reactor	393.16 K

5. RESULTS & DISCUSSION

The MPC methodology explained in Part 3 will be applied to CSTR defined and derived in Part 4. The controller design, tuning and performance analysis with traditional controllers will be represented in this section.

5.1 Control Strategy

In the control strategy for the CSTR defined in the previous section for propylene glycol production, concentration of the product propylene glycol (C_C) and the temperature of the reactor (T) are considered to be controlled variables. Between these two controlled variables, reactor temperature will be the measured input to the system. The controlled variables are considered to be manipulated by propylene oxide – methanol mixture flow rate (F_A) and coolant flow rate (F_{CW}). Beyond that multi input – multi output (MIMO) structure, initial concentration of propylene oxide (C_{Ai}) and coolant temperature (T_{a1}) are considered as measured disturbances. The flow of control of CSTR is shown in Figure 5.1.

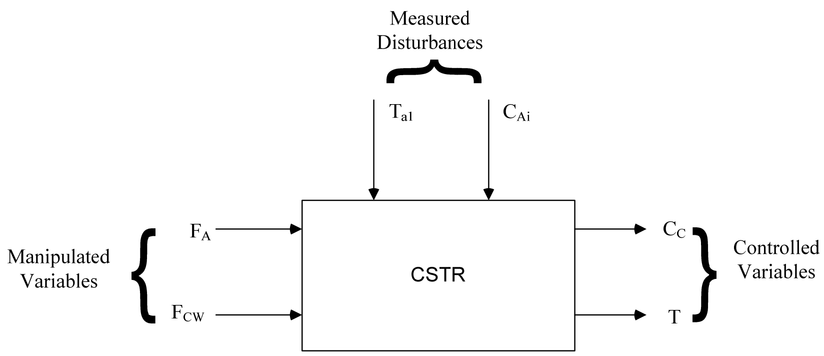


Figure 5.1: Propylene glycol production control diagram.

5.2 Step Response Models

Step responses are aimed to be obtained and used in the MPC design. To do so, open loop responses of controlled variables are obtained by giving step changes to the manipulated variables. These step response coefficients are than utilized in order to obtain the process condition by singular value decomposition method. Also step responses of measured disturbances are also obtained.

Open loop responses of controlled variables, concentration of the product propylene glycol (C_C) and the temperature of the reactor (T) for a step change in manipulated variables propylene oxide – methanol mixture flow rate (F_A) and coolant flow rate (F_{CW}) are given between Figure 5.2 and Figure 5.5.

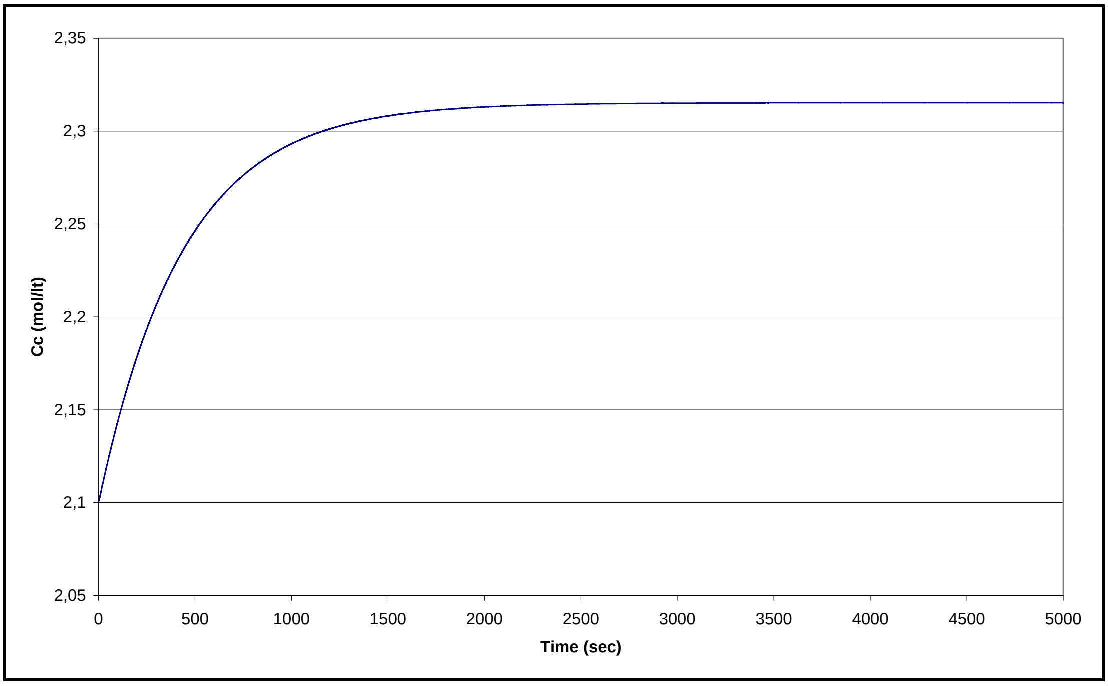


Figure 5.2: Open loop step response of propylene glycol concentration C_C for a 10 % step change in ethylene oxide – methanol mixture (F_A) from 0.733 lt/sec to 0.8063 lt/sec.

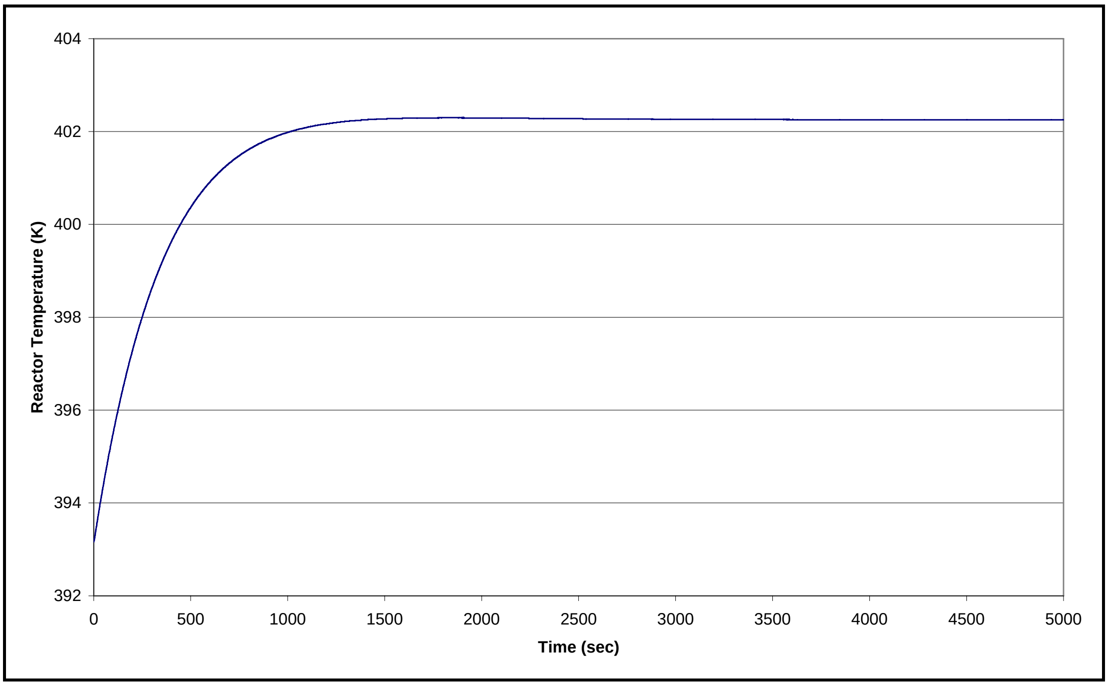


Figure 5.3: Open loop step response of reactor temperature for a 10 % step change in ethylene oxide – methanol mixture (F_A) from 0.733 lt/sec to 0.8063 lt/sec.

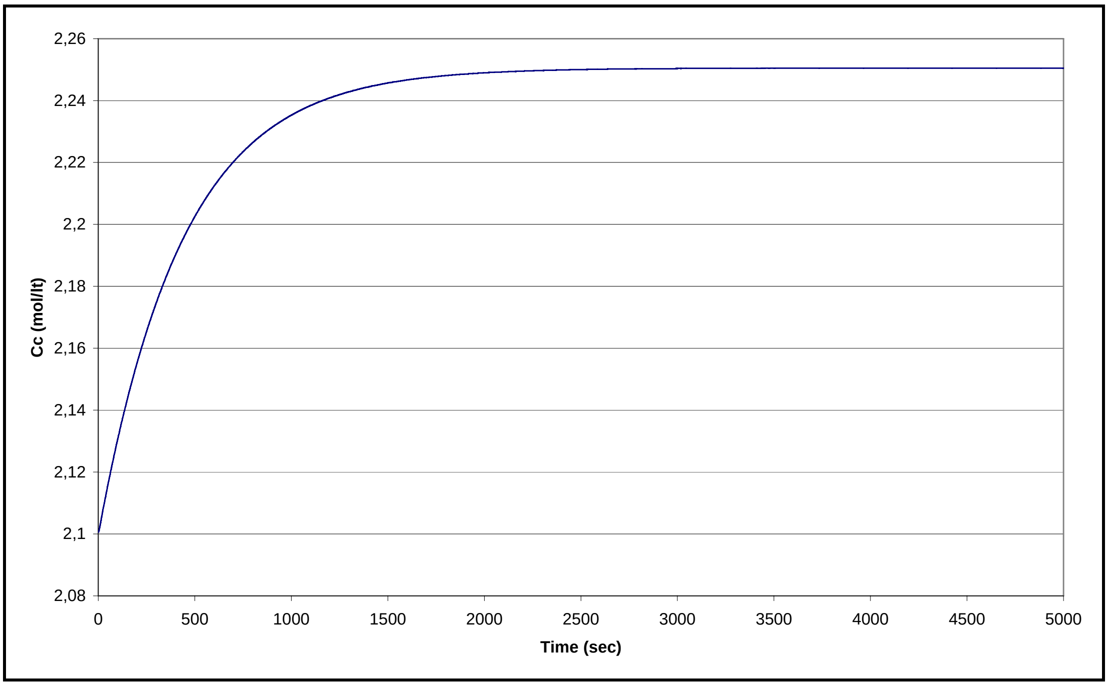


Figure 5.4 Open loop step response of propylene glycol concentration C_C for a 10 % step change in coolant flow rate (F_{CW}) from1.833 lt/sec to 2.0163 lt/sec.

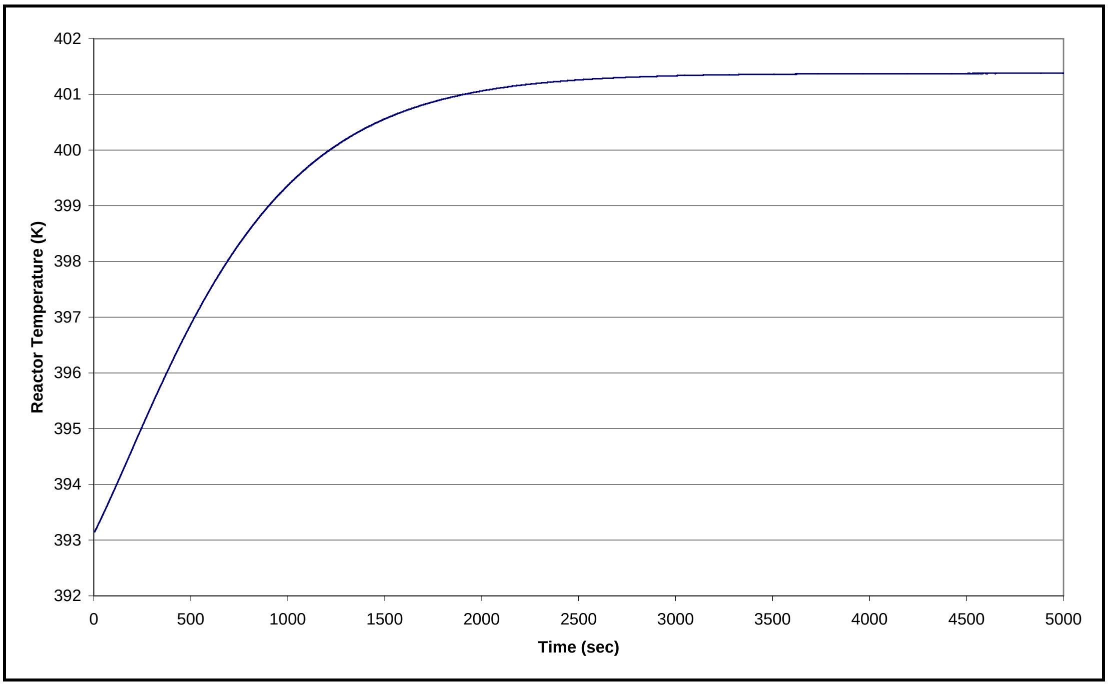


Figure 5.5 Open loop step response of reactor temperature for a 10 % step change in coolant flow rate (F_{CW}) from1.833 lt/sec to 2.0163 lt/sec.

Using the step responses steady state gain matrix is obtained. This matrix is then subject to Singular Value Decomposition method, and the condition number is found to be 567, which shows a poor-conditioned system and necessitates the use of a MIMO-MPC design.

Open loop responses of controlled variables, concentration of the product propylene glycol (C_C) and the temperature of the reactor (T) also for a step change in measured disturbances initial concentration of propylene oxide (C_{Ai}) and initial temperature of coolant (T_{a1}) are given between Figure 5.6 and Figure 5.9.

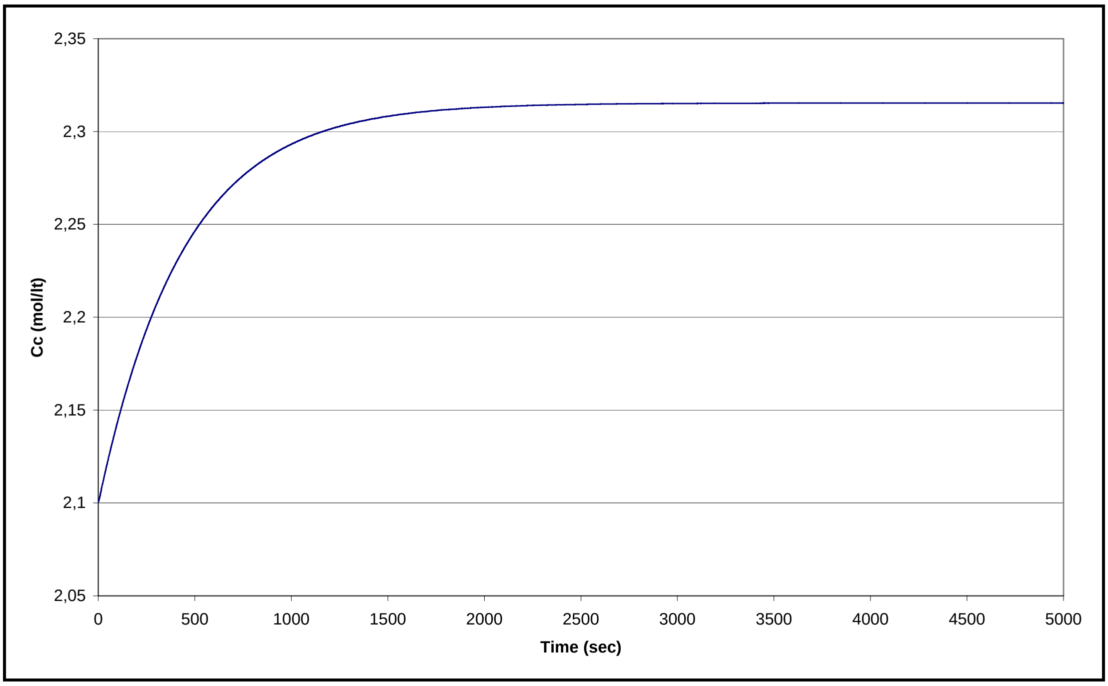
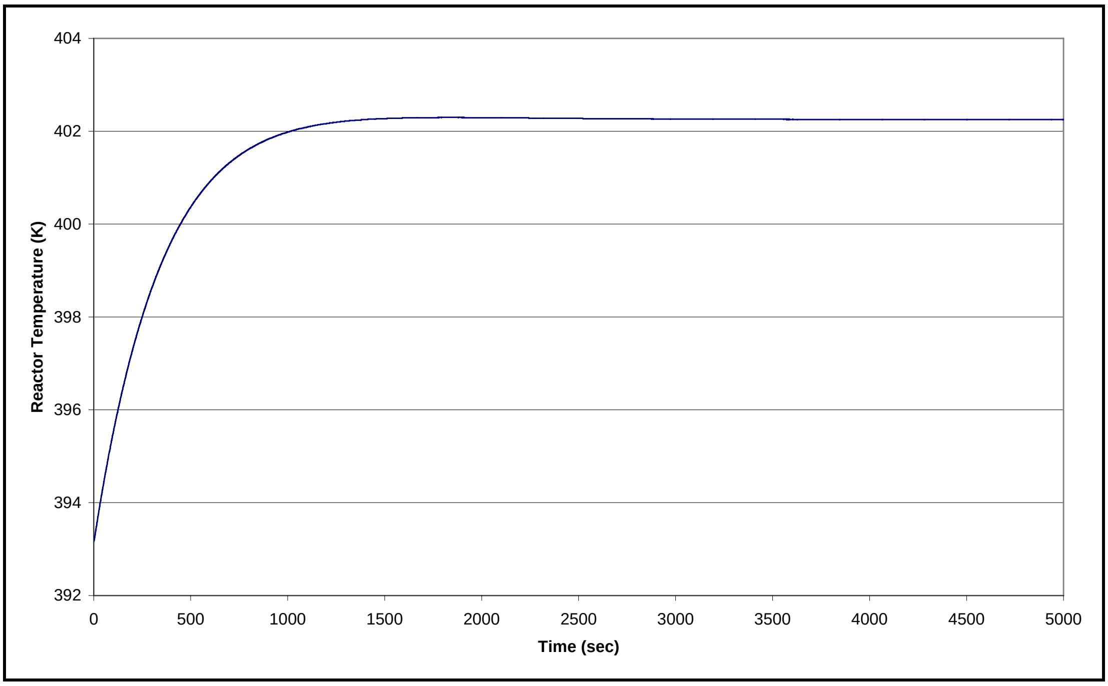


Figure 5.6 Open loop step response of propylene glycol concentration C_C for a 10 % step change in initial propylene oxide concentration (C_{Ai}) from7.39 mol/lt to 8.129 mol/lt.



.**Figure 5.7** Open loop step response of reactor temperature for a 10 % step change in initial propylene oxide concentration (C_{Ai}) from7.39 mol/lt to 8.129 mol/lt.

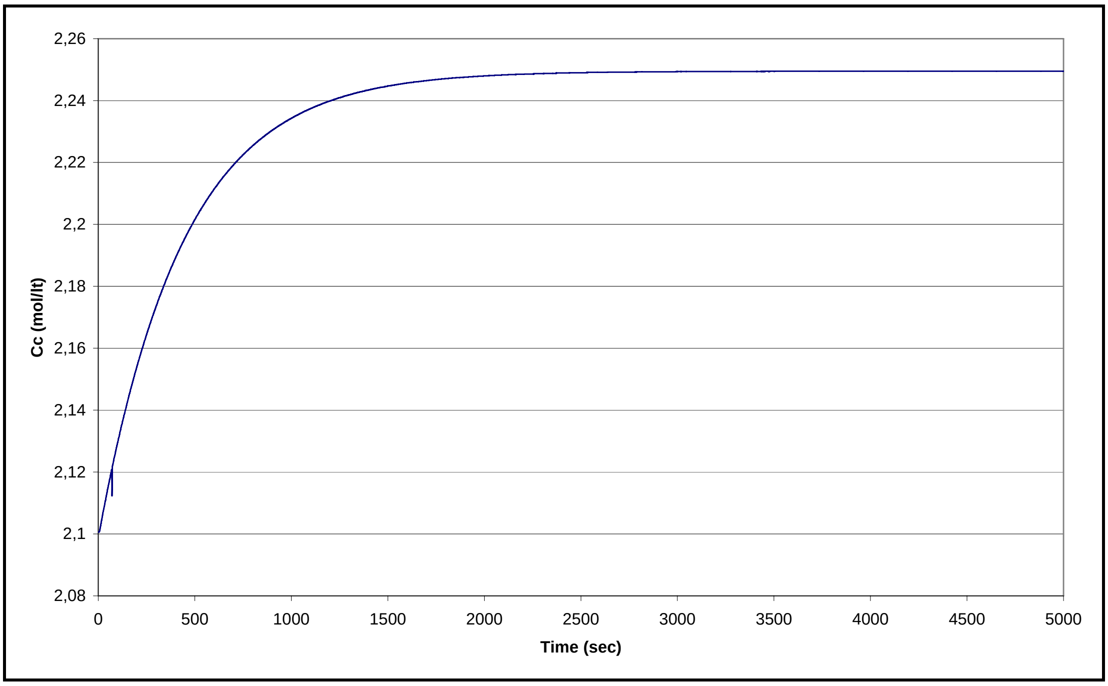


Figure 5.8 Open loop step response of propylene glycol concentration C_C for a 2 K step change in coolant initial temperature (T_{a1}) from 293 K to 295 K.

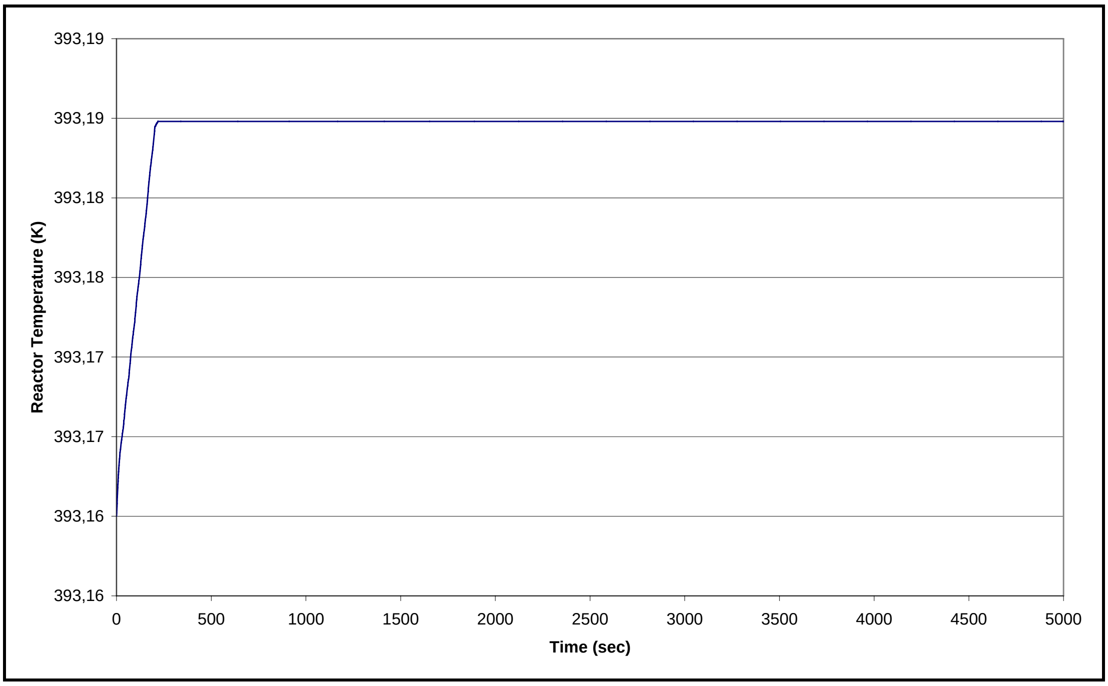


Figure 5.9 Open loop step response of reactor temperature for a 2 K step change in coolant initial temperature (T_{a1}) from 293 K to 295 K.

5.3 Design of MIMO – MPC

After examining open-loop responses of controlled variables to step changes, a multi input – multi output MPC model is developed in which propylene oxide – methanol mixture flow rate (F_A) and coolant flow rate (F_{CW}) are manipulated variables, concentration of the product propylene glycol (C_C) and the temperature of the reactor (T) are controlled variables and initial concentration of propylene oxide (C_{Ai}) and coolant temperature (T_{a1}) are measured disturbances. Using the design equations and step response curves, the controller is developed and tested. Control algorithm is written in MATLAB. Also MPC toolbox of MATLAB code is improved to adjust problem definition.

In order to determine the model horizon, open loop responses are examined. When Figure 5.3 is examined, it can be seen that propylene glycol concentration reaches 99 % completion in about 2600 sec. Dividing the completion time with sampling time of 10 seconds gives 260 as the model horizon (M). Prediction horizon is selected as 85 % of model horizon as a rule of thumb as 221.

Tuning of the developed MPC is carried out by manipulating weighting matrices $f(\lambda_1/ \lambda_2)$ and control horizon (C).

5.4 MPC Performance in Set Point Tracking

The developed MPC is tested for set point tracking. First by taking a fixed control horizon, responses and integral absolute error (IAE) scores are examined. As fixed control horizon, 60 % of model horizon is selected as 156. The set point of propylene glycol (C_C) is increased at a magnitude of 5 % from 2.1006 mol/lt to 2.2056 at 1000th second, and decreased at a magnitude of 10 % from 2.2056 to 1.9850 mol/lt at 3500th second. The performance of MPC for set point tracking is shown for different values of rate weights, 0.1, 0.05, 0.01, 0.005 and 0.001 at Figure 5.10.

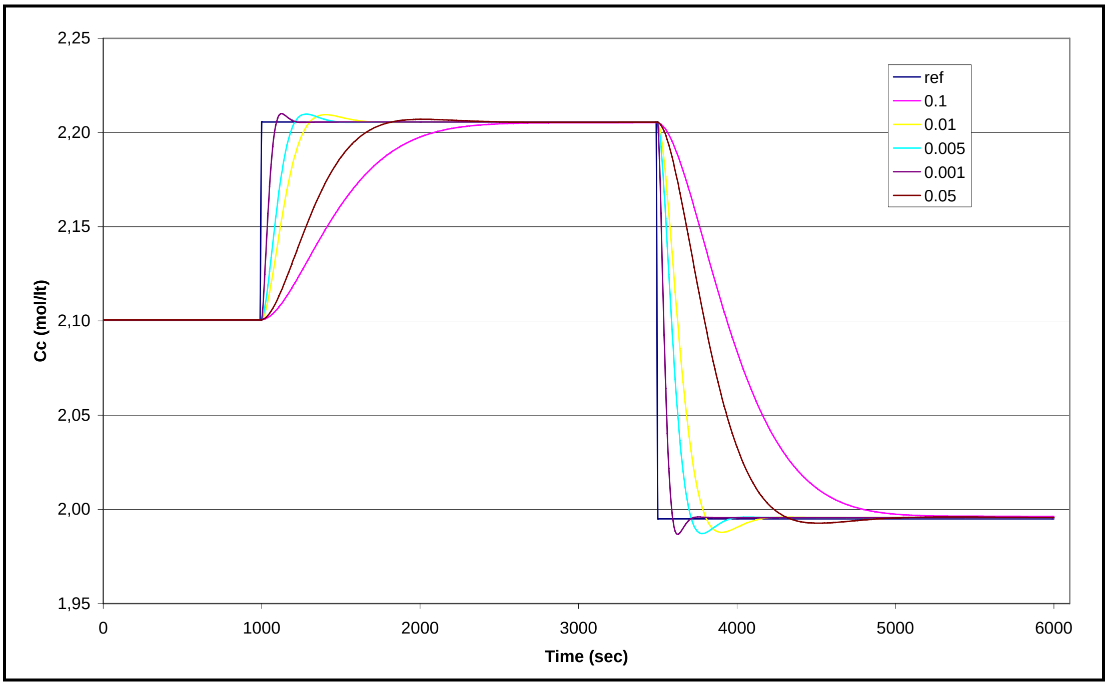
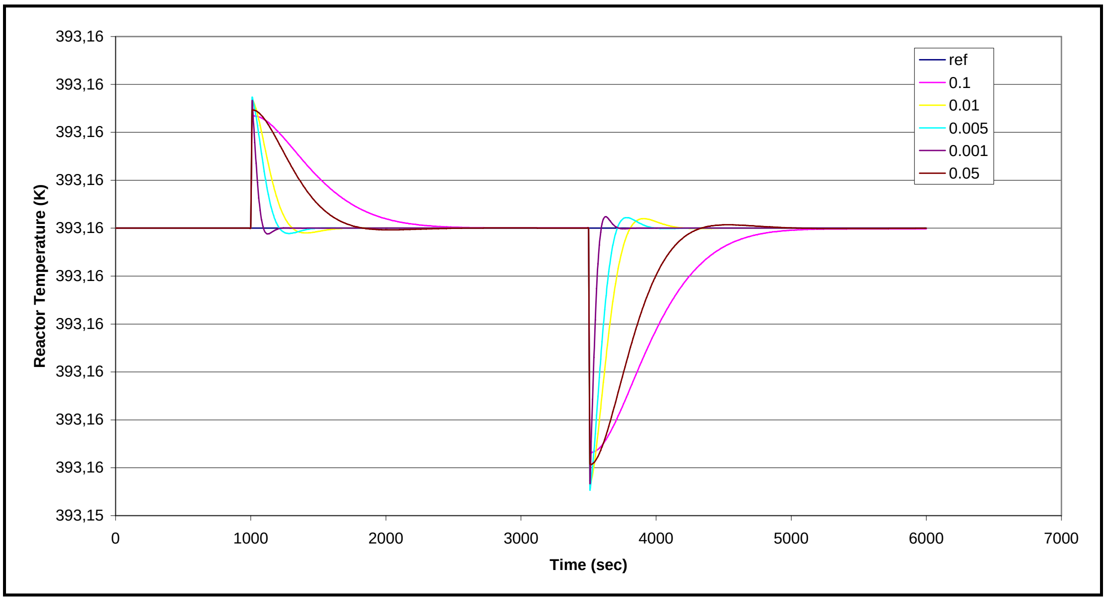


Figure 5.10 : Response of C_C to a 5 % increase in the set point of C_C followed by 10 % decrease in the set point of C_C for different f values.

The responses of reactor temperature (T), propylene oxide – methanol mixture flow rate (F_A) and coolant flow rate (F_{CW}) for C_C concentration set point tracking is given in Figures 5.11 to 5.13.



.**Figure 5.11 :** Response of T to a 5 % increase in the set point of C_C followed by 10 % decrease in the set point of C_C for different f values.

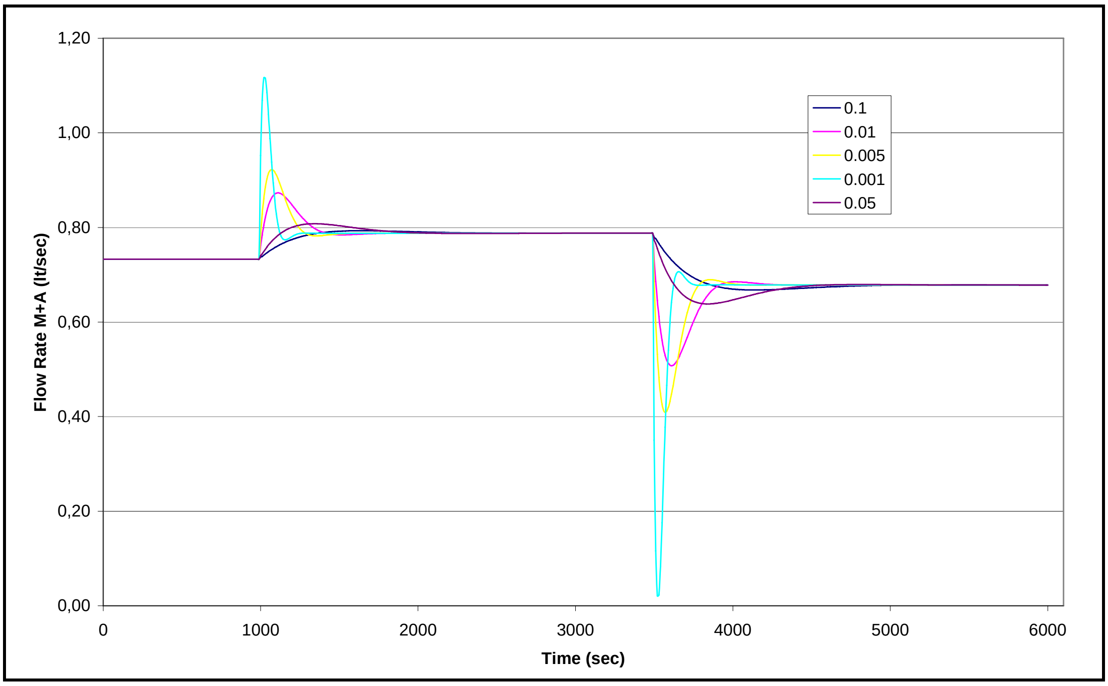


Figure 5.12 : Response of F_A to a 5 % increase in the set point of C_C followed by 10 % decrease in the set point of C_C for different f values.

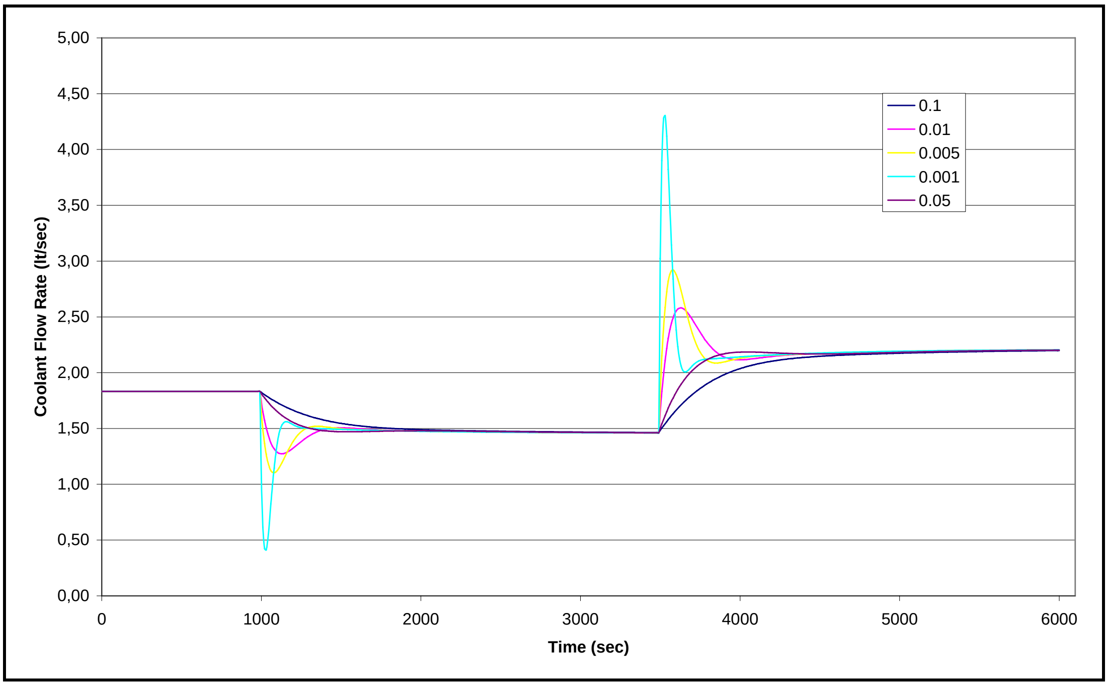


Figure 5.13 : Response of F_{CW} to a 5 % increase in the set point of C_C followed by 10 % decrease in the set point of C_C for different f values.

IAE scores for set point tracking for different f values is given in Table 5.1.

Table 5.1: IAE scores of C_C set point tracking for different f values at C=156.

Value of f	IAE Score
0.1	53.073
0.05	34.542
0.01	13.632
0.005	9.540
0.001	4.418

Although IAE score improves as f value decreases, high peaks occur with f=0.005 in coolant and reactant flow rates at these small values. Therefore the best f value is chosen to be f=0.01.

In order to observe the effect of control horizon (C), different values of C values are tested as a percentage of model horizon for f=0.01. Figure 5.14 represents responses of the system for set point tracking at different C values.

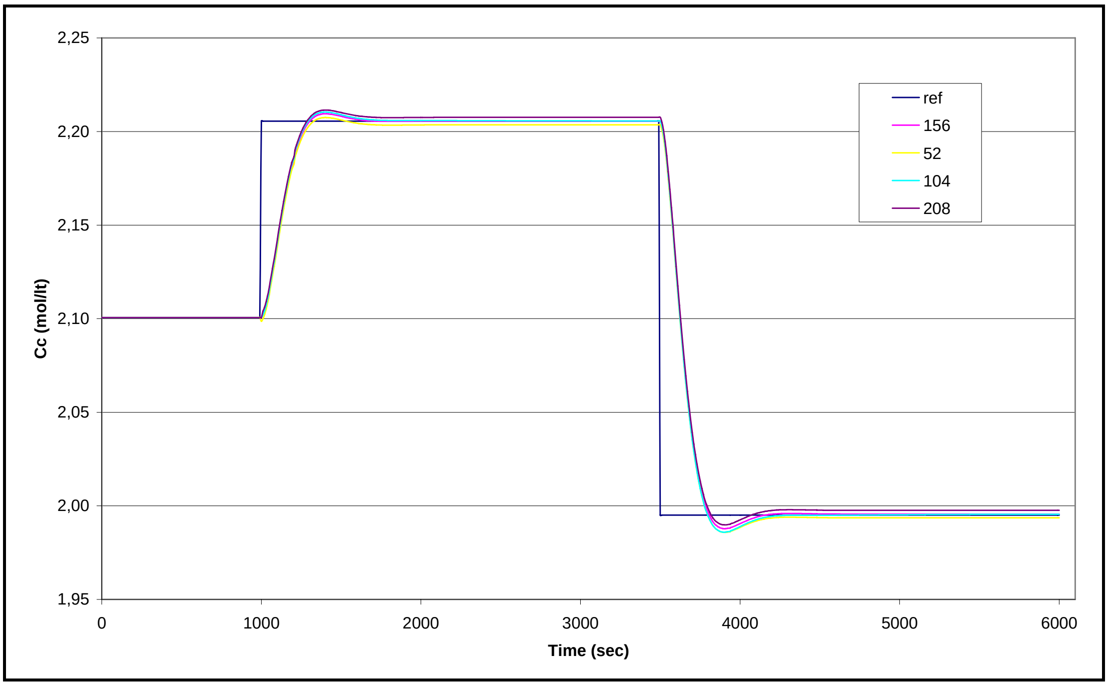


Figure 5.14 : Response of C_C to a 5 % increase in the set point of C_C followed by 10 % decrease in the set point of C_C for different C values.

The responses of reactor temperature (T), propylene oxide – methanol mixture flow rate (F_A) and coolant flow rate (F_{CW}) for C_C concentration set point tracking at different C values is given in Figures 5.14 to 5.16.

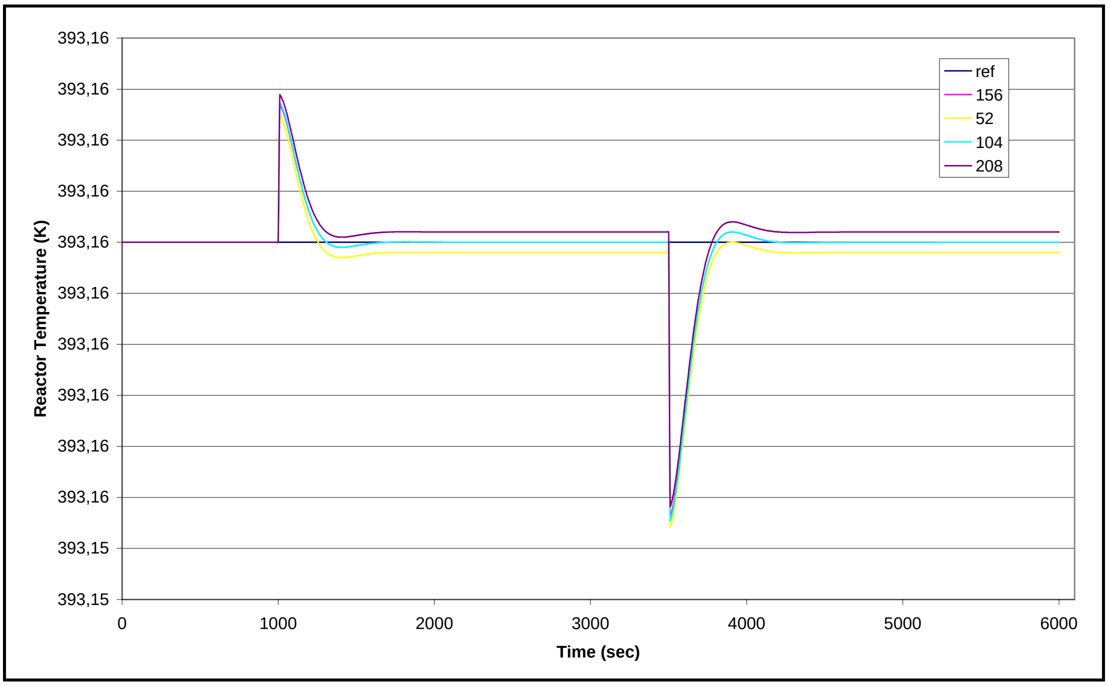


Figure 5.15 : Response of T to a 5 % increase in the set point of C_C followed by 10 % decrease in the set point of C_C for different f values.

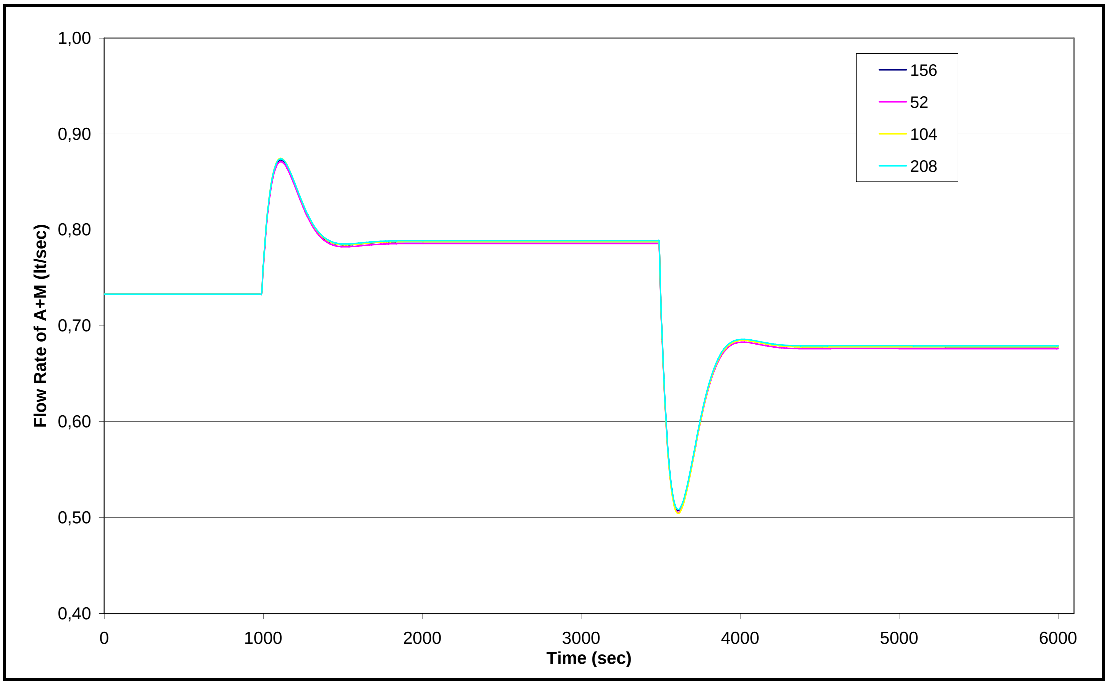


Figure 5.16 : Response of F_A to a 5 % increase in the set point of C_C followed by 10 % decrease in the set point of C_C for different f values.

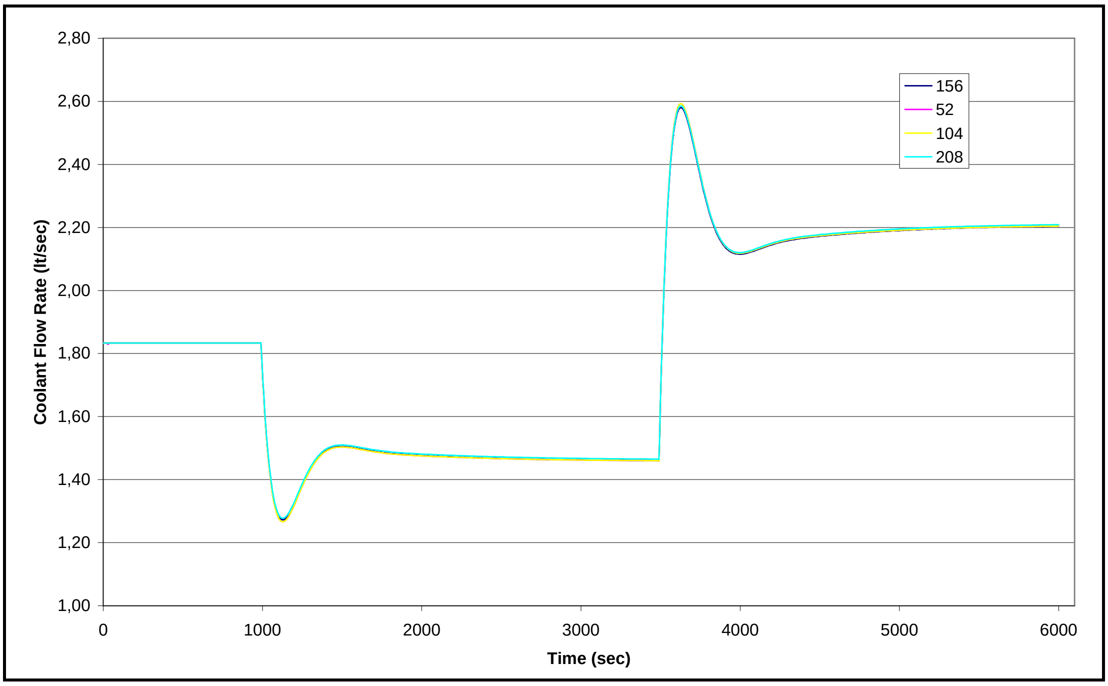


Figure 5.17 : Response of F_{CW} to a 5 % increase in the set point of C_C followed by 10 % decrease in the set point of C_C for different f values.

IAE scores for set point tracking at different control horizons is given in Table 5.2.

Table 5.2: IAE scores of C_C set point tracking for different C values at f=0.01.

Value of C	IAE Score
52 (20 % of M)	13.978
104 (40 % of M)	13.442
156 (60 % of M)	13.632
208 (80 % of M)	14.214

Although there is not big difference in IAE scores, there exists a slight difference from set point for C=52 and C=208. So C=156 is chosen as the best case. In overall evaluation, f = 0.01 and C = 156 is chosen as the best case.

5.5 MPC Performance in Disturbance Rejection

Disturbance rejection performance of the developed MPC (f = 0.01 and C=156) is tested by manipulating measured disturbances; initial concentration of propylene oxide (C_{Ai}) and coolant temperature (T_{a1}) and expected to control for propylene glycol (C_c) and temperature set points.

In the first case a disturbance of 10 % increase in the initial concentration of propylene oxide (C_{Ai}) from 7.39 mol/lt to 8.13 mol/lt at 1000th second. Figure 5.17 to Figure 5.20 represent the response of the system for changes in product concentration C_C, reactor temperature (T), propylene oxide – methanol mixture flow rate (F_A) and coolant flow rate (F_{CW}).

Although there response of C_C is fast, there is a 2.4 % offset with IAE score of 22.34. Same deviation can be observed in temperature of the reactor with 0.04 %.

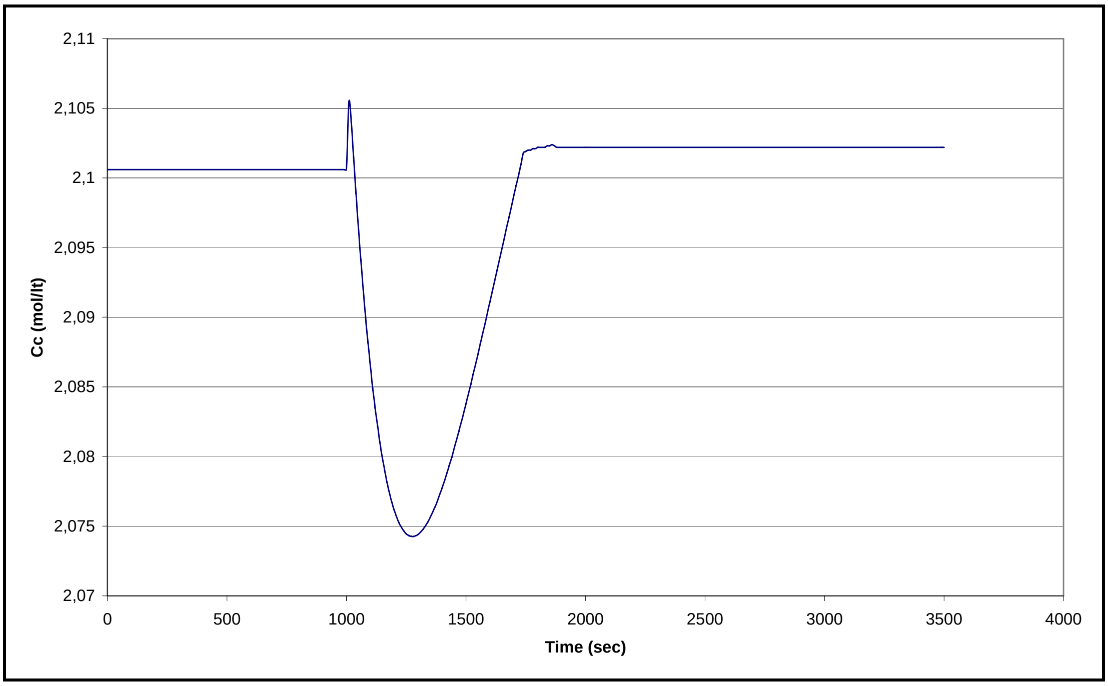


Figure 5.18 : Response of C_c to a 10 % increase in the initial concentration of propylene oxide.

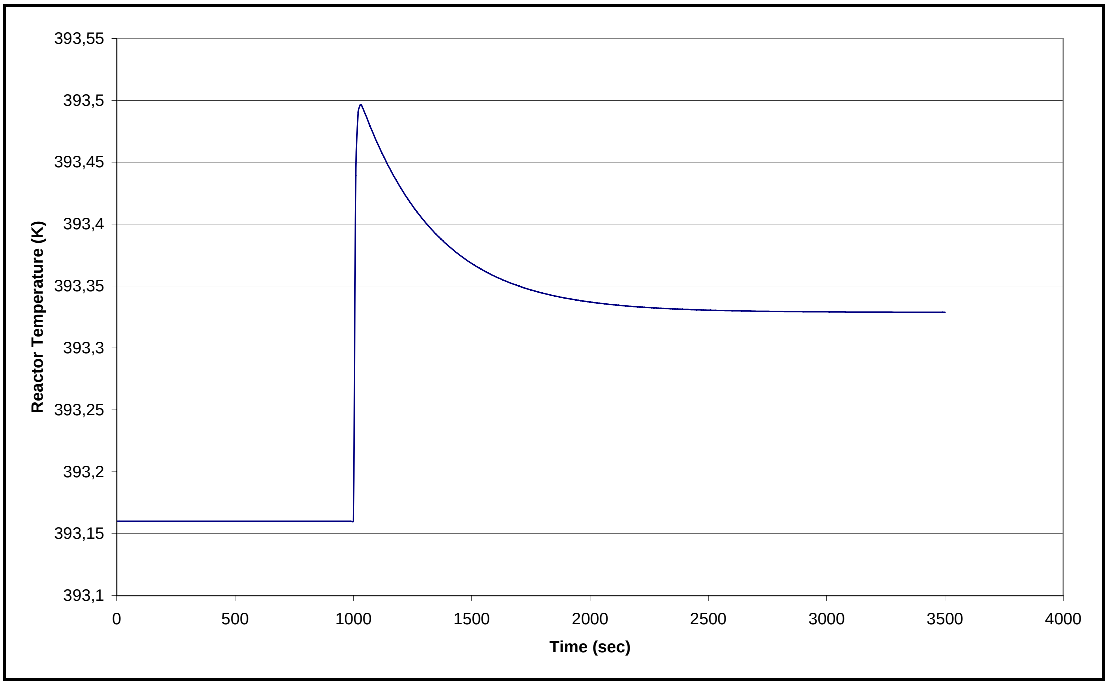


Figure 5.19 : Response of T to a 10 % increase in the initial concentration of propylene oxide.

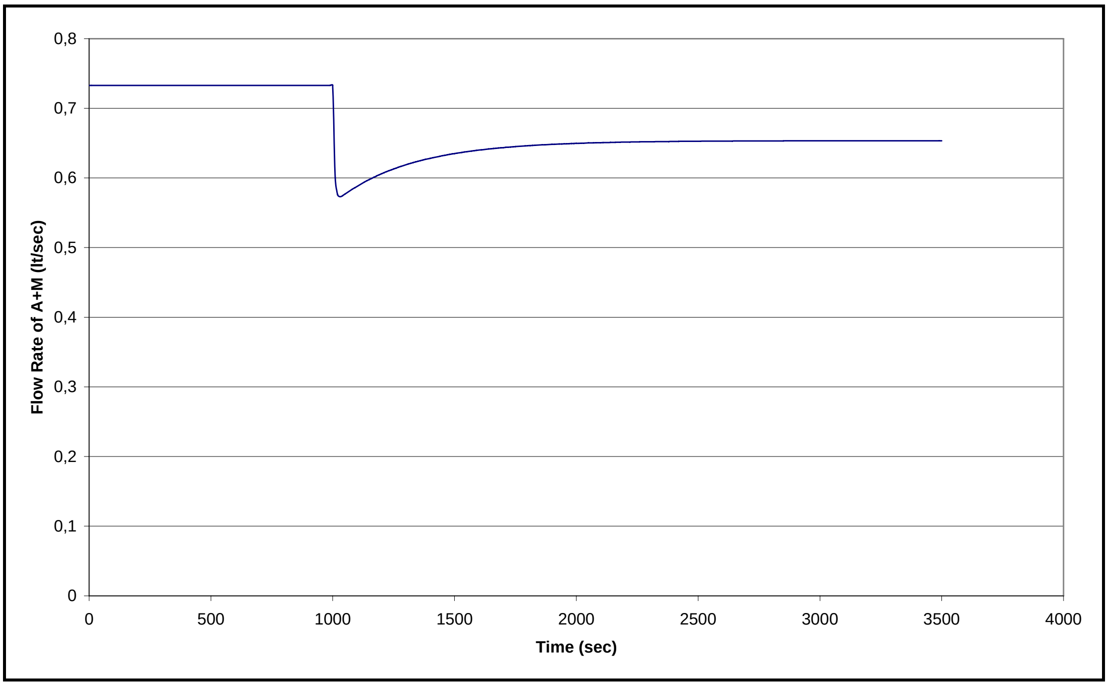


Figure 5.20 : Response of F_A to a 10 % increase in the initial concentration of propylene oxide.

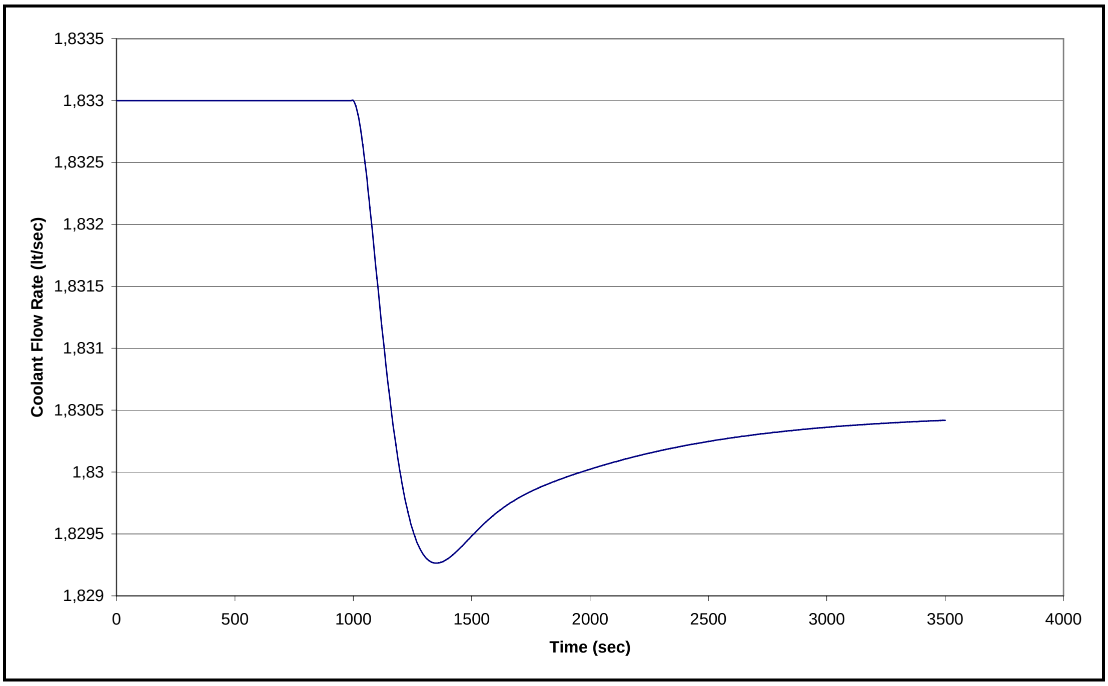


Figure 5.21 : Response of F_{CW} to a 10 % increase in the initial concentration of propylene oxide.

In order to observe the controller's performance in disturbance rejection, a change of 2 Kelvin in the coolant temperature is applied to the process at 1000^{th} second. Figure 5.21 to Figure 5.24 shows the responses of the system for changes in product concentration C_C, reactor temperature (T), propylene oxide – methanol mixture flow rate (F_A) and coolant flow rate (F_{CW}).

Both responses to C_C concentration and temperature are successful with IAE scores of 10.41 and 8.71, respectively.

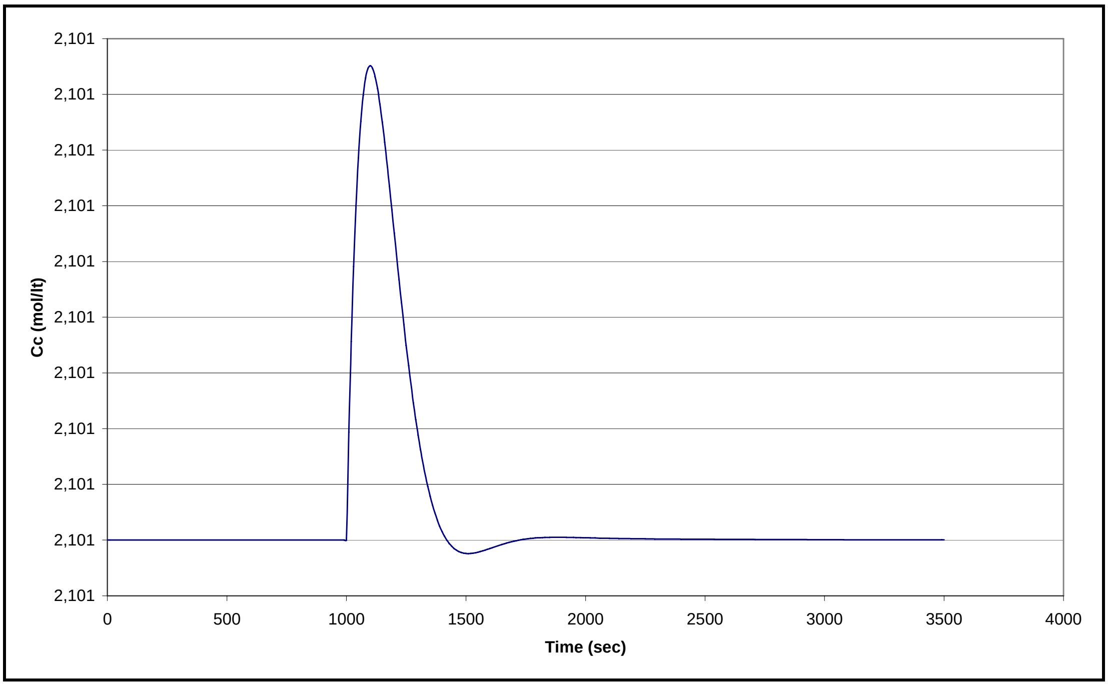


Figure 5.22 : Response of C_c to a 2 K increase in the coolant temperature.

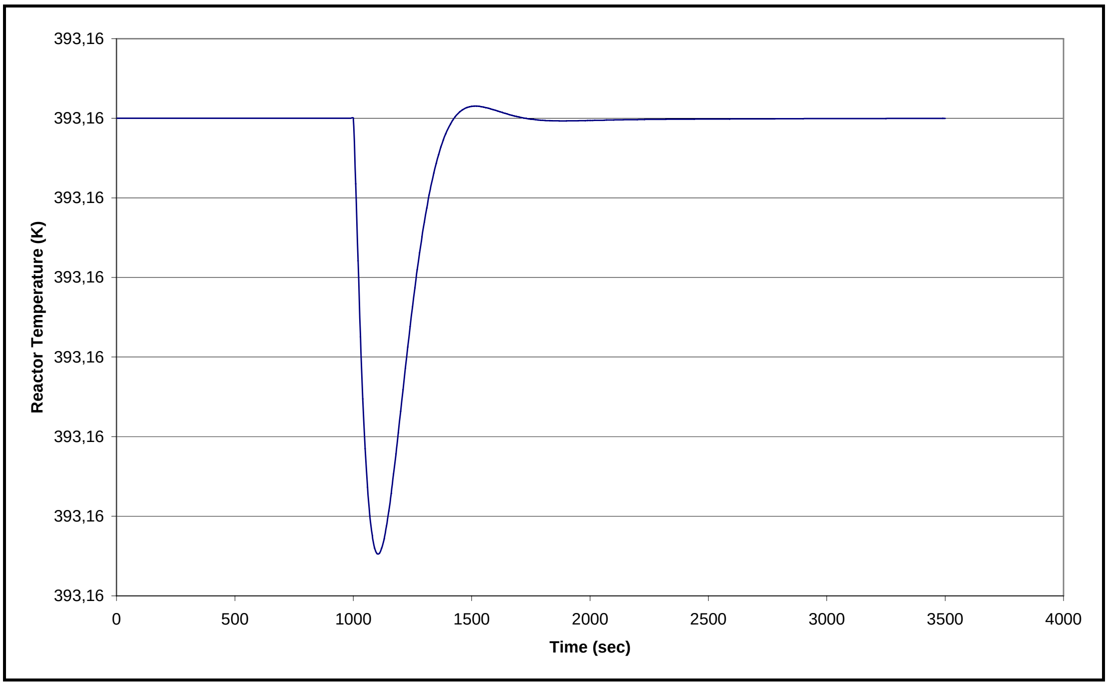


Figure 5.23 : Response of T to a 2 K increase in the coolant temperature.

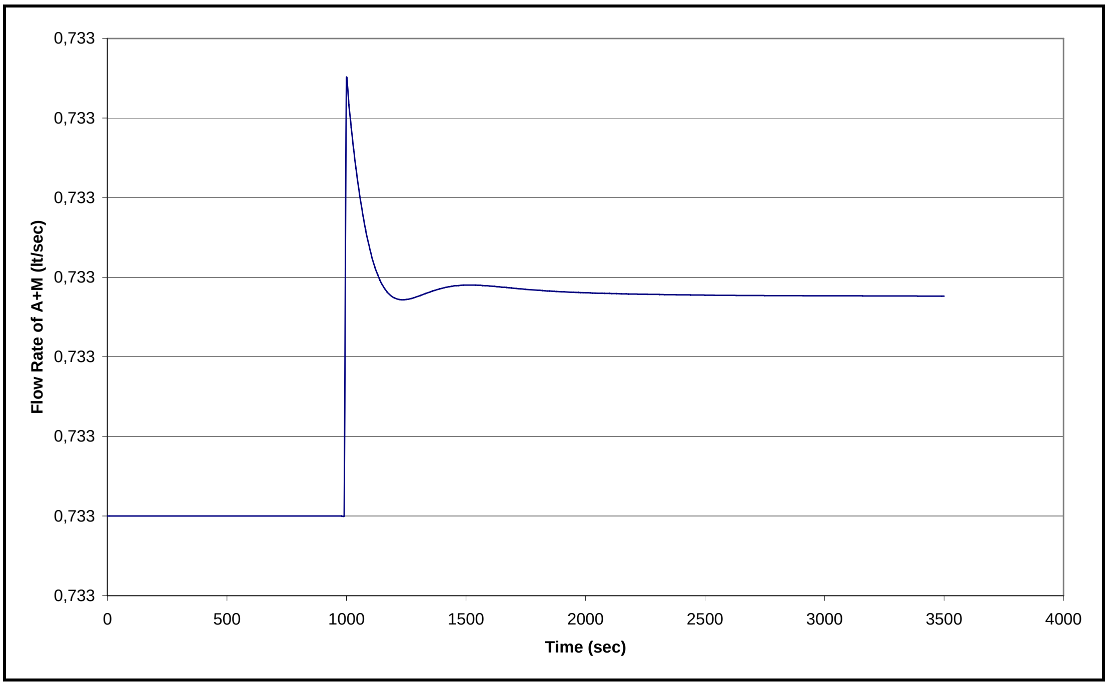


Figure 5.24 : Response of F_A to a 2 K increase in the coolant temperature.

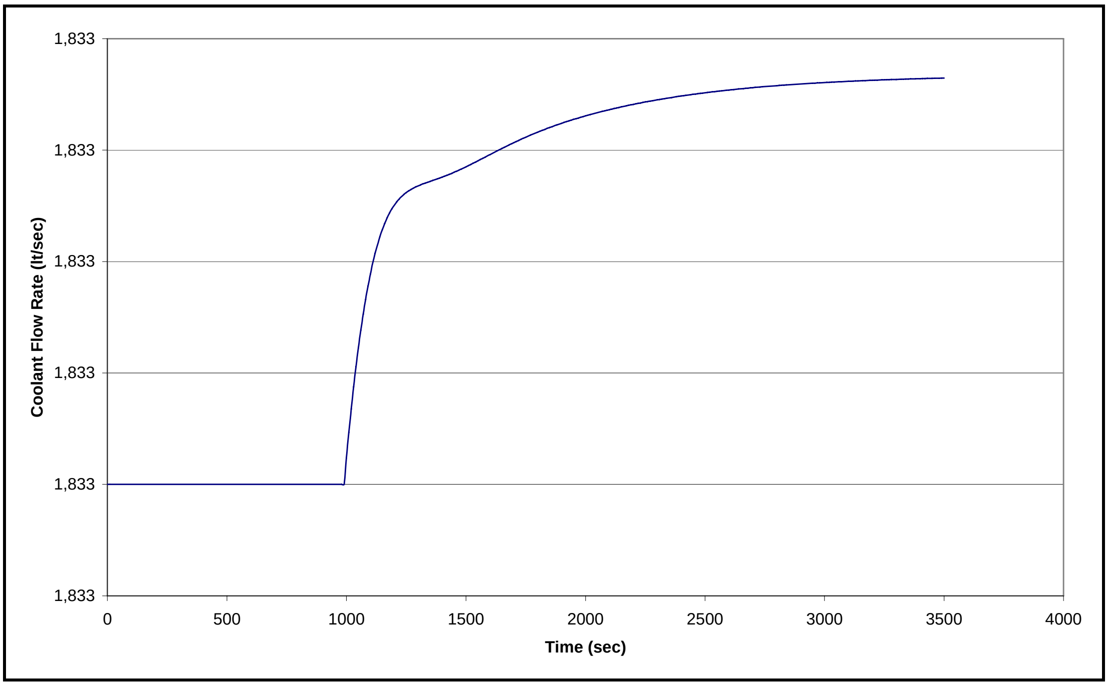


Figure 5.25 : Response of F_{CW} to a 2 K increase in the coolant temperature.

5.6 MPC Performance for Robustness

Robustness is defined by Seborg et al., (1989) as the controller's insensitivity to changes in process conditions and to errors in the assumed process model. For the sake of analyzing controller robustness, a 10 % change in the reaction rate constant from k_0= 4.711*10^9 sec^{-1} to 5.182*10^9 sec^{-1}. After changing such a process parameter, steady state values are reevaluated as C_{Ass}=0.0086 mol/lt, C_{Bss}=37.308 mol/lt, C_{Mss}=3.5279 mol/lt, C_{Css}=2.1024 mol/lt and T_{ss}=393.24 K. Using these values step responses are also reevaluated.

Set point tracking is examined for the new data for set point changes of 5 % increase at 1000^{th} second and 10 % decrease of set point of propylene glycol (C_C) at 3500^{th} second, while rate weight f = 0.01 and control horizon C = 156. The responses of propylene glycol (C_C) and reactor temperature (T) with propylene oxide – methanol mixture flow rate (F_A) and coolant flow rate (F_{CW}) is presented in Figure 5.25 to Figure 5.28. Successful tracking is obtained with IAE score of 15.41.

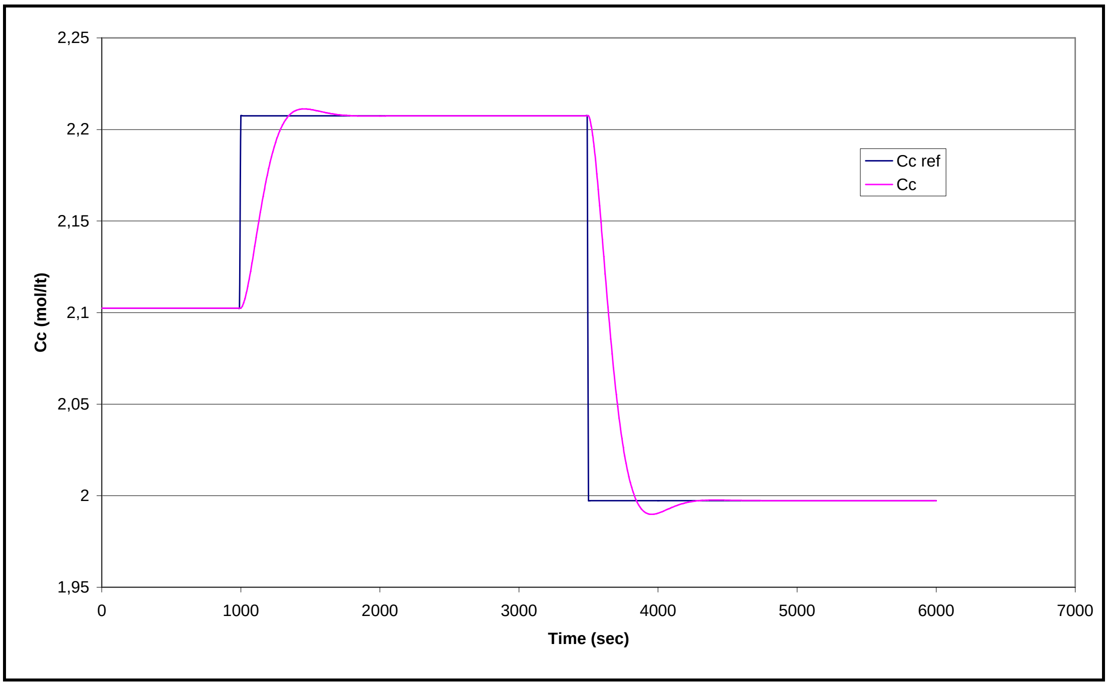


Figure 5.26: Response of C_c to set point change.

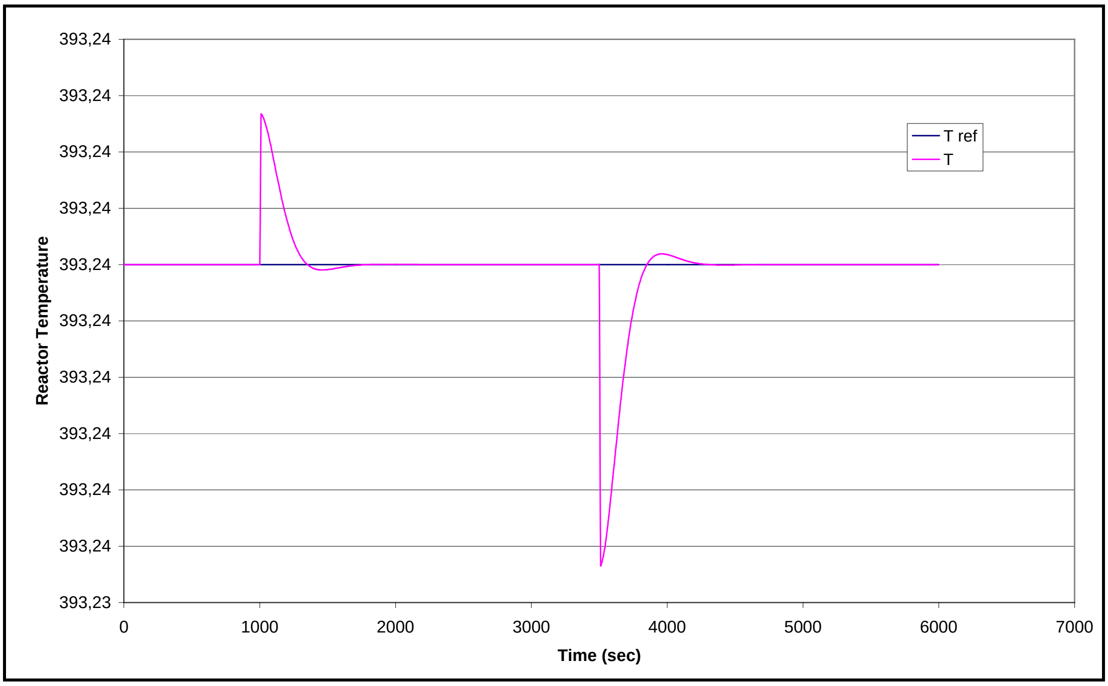


Figure 5.27: Response of T to set point change.

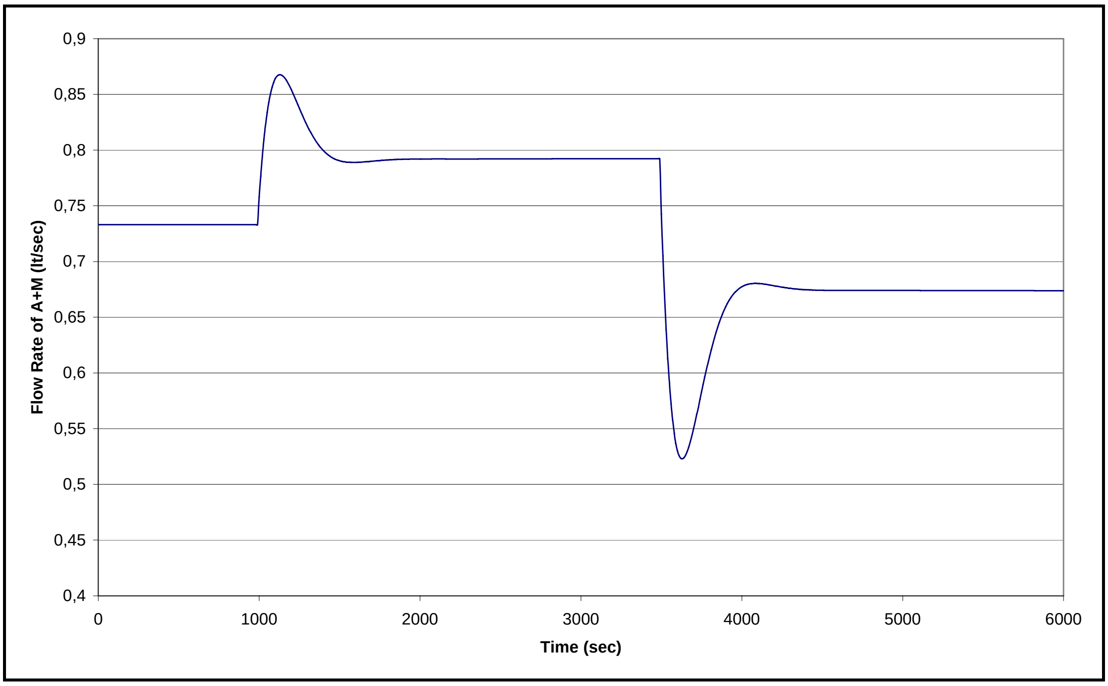


Figure 5.28: Response of F_A to set point change.

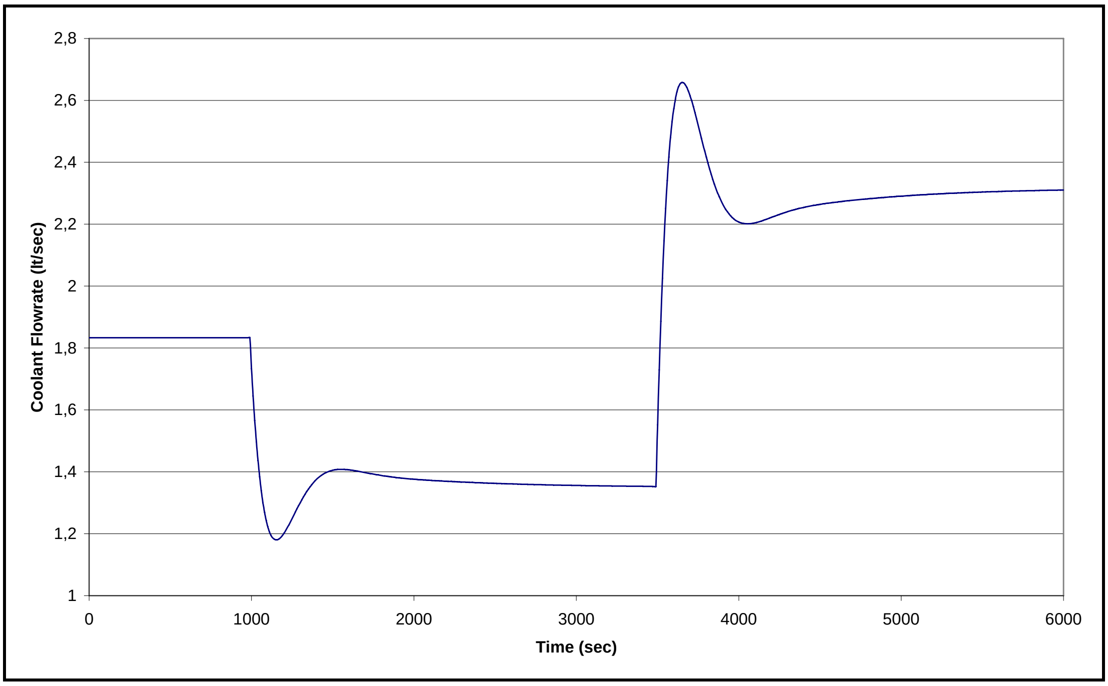


Figure 5.29: Response of F_{CW} to set point change.

Performance of MPC controller with new process conditions is also evaluated with disturbance rejection. A disturbance of 10 % increase in the initial concentration of propylene oxide (C_{Ai}) from 7.39 mol/lt to 8.13 mol/lt at 1000th second. Figure 5.29 to Figure 5.32 shows the response of the system for changes in product concentration C_C, reactor temperature (T), propylene oxide – methanol mixture flow rate (F_A) and coolant flow rate (F_{CW}). IAE score is obtained as 13.85.

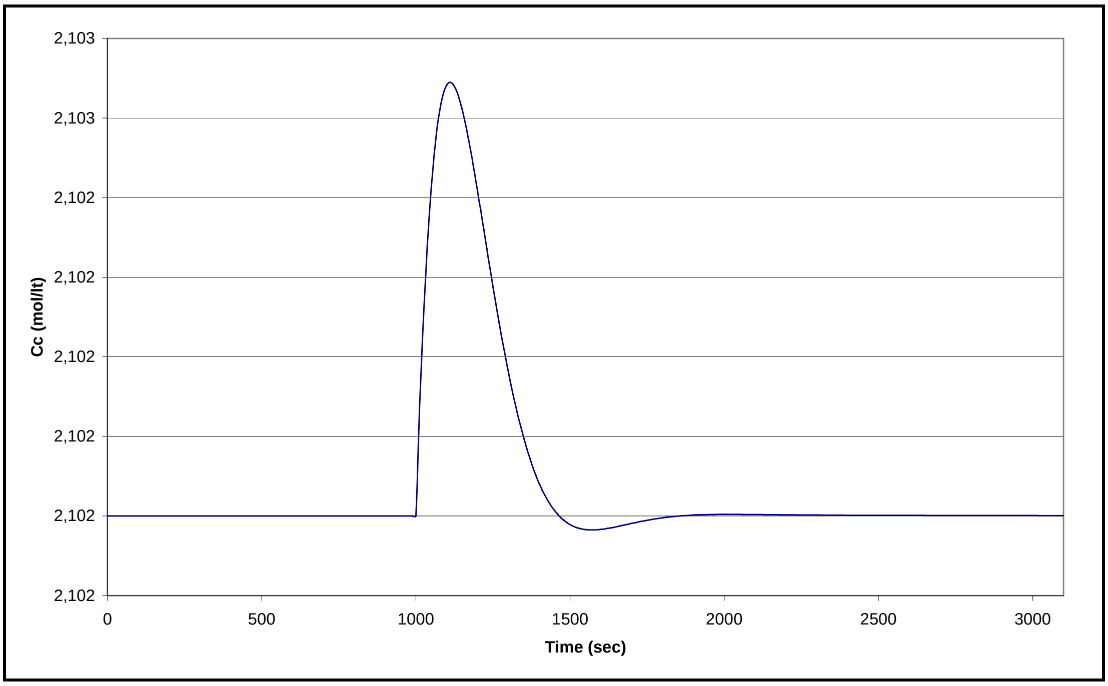


Figure 5.30 : Response of C_c to disturbance rejection.

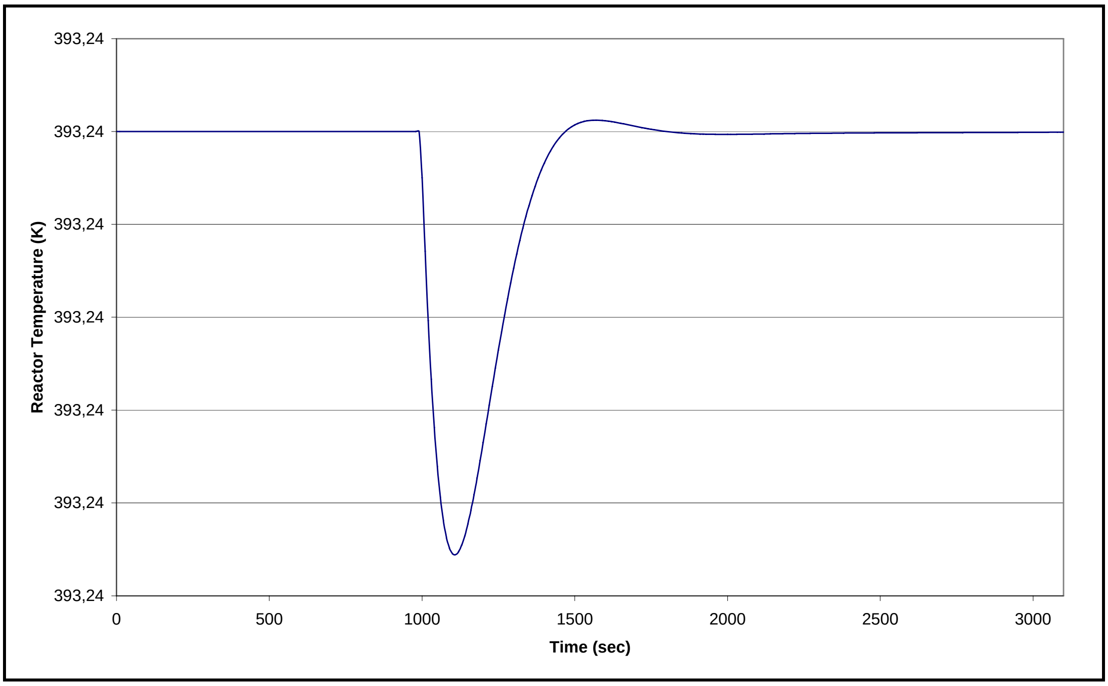


Figure 5.31 : Response of T to disturbance rejection.

Figure 5.32 : Response of F_A to disturbance rejection.

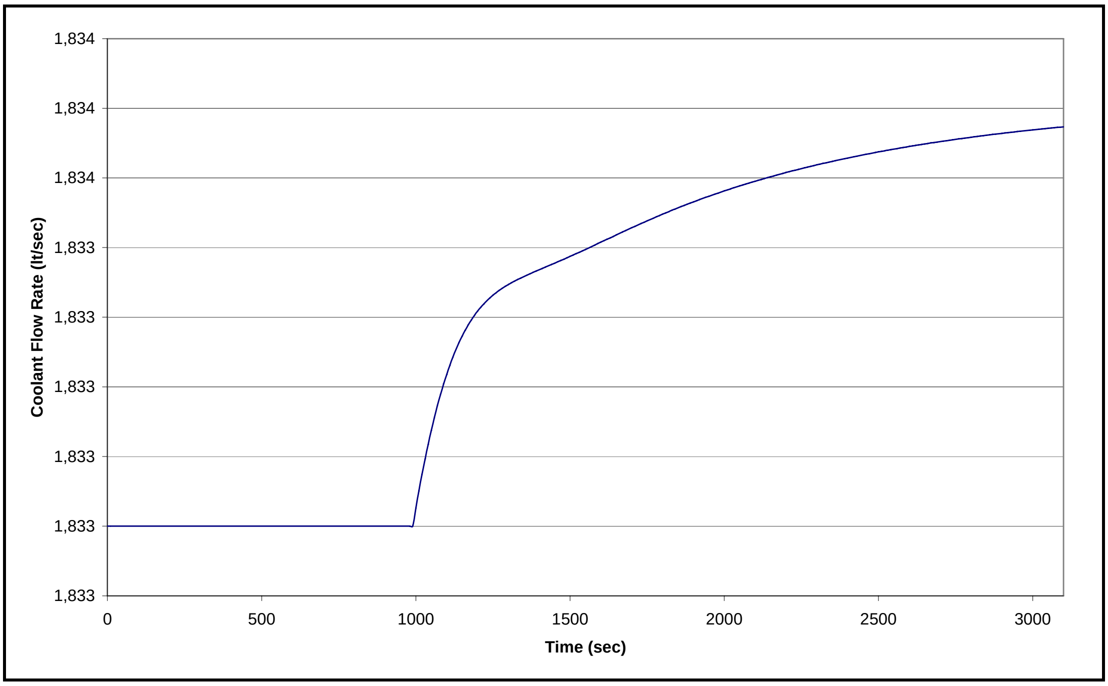


Figure 5.33 : Response of F_{CW} to disturbance rejection.

As the second case, disturbance of 2 Kelvin increase in the coolant temperature is analyzed. Figure 5.33 to Figure 5.36 shows the response of the system for changes in product concentration C_C, reactor temperature (T), propylene oxide – methanol mixture flow rate (F_A) and coolant flow rate (F_{CW}). The IAE score is obtained as 8.21.

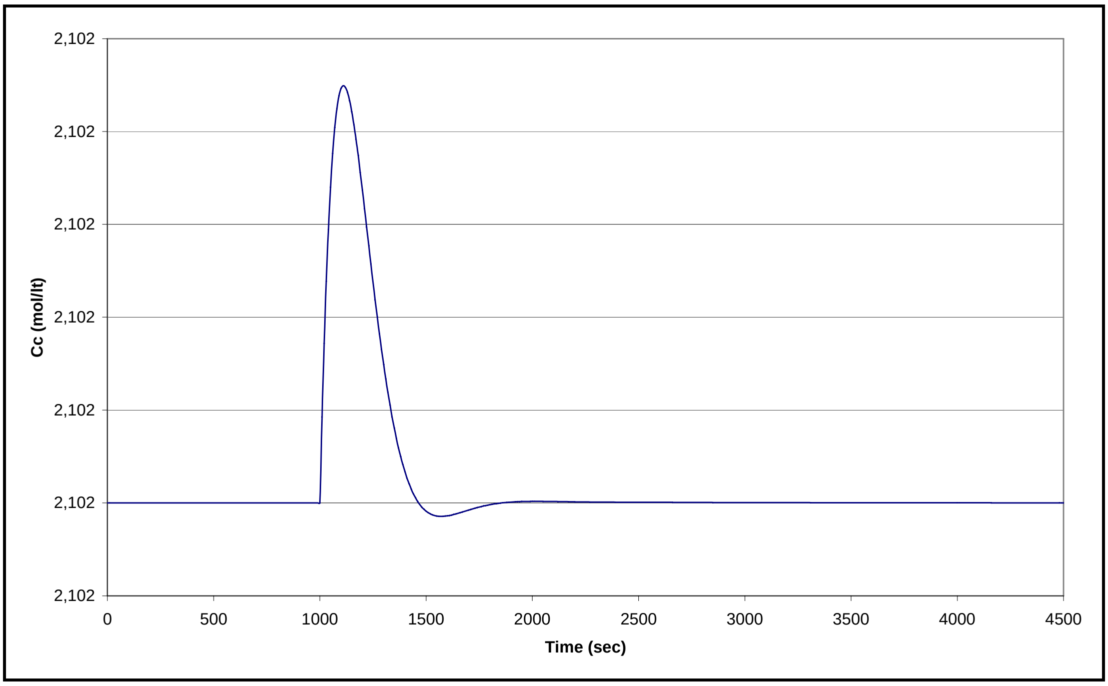


Figure 5.34 : Response of C_c to disturbance rejection.

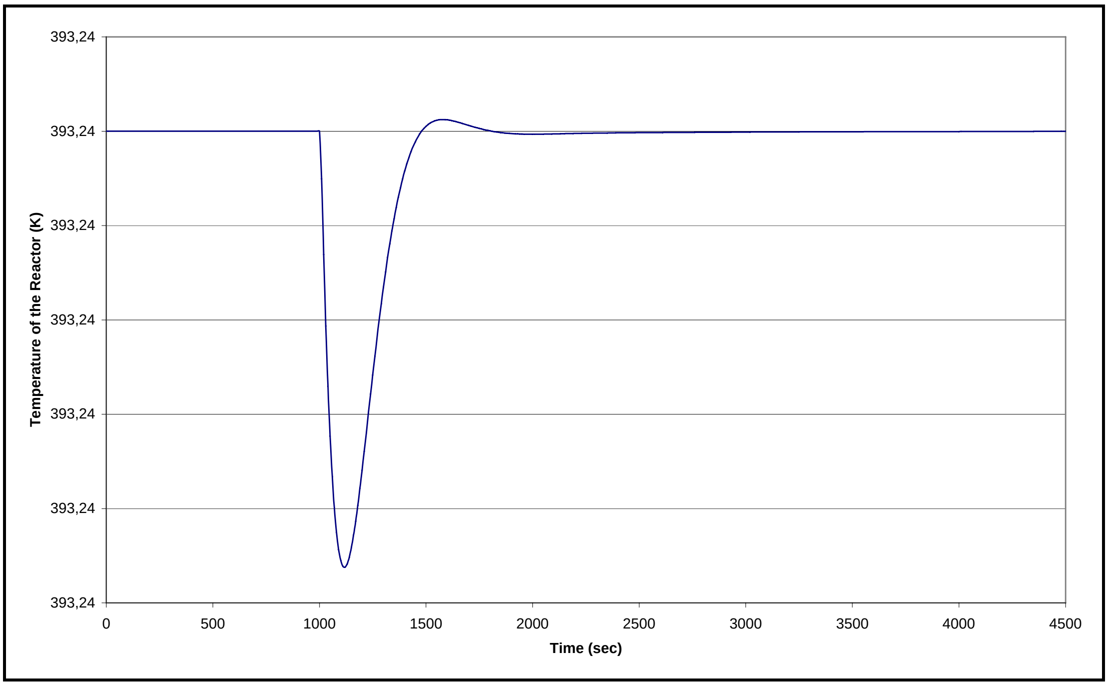


Figure 5.35 : Response of T to disturbance rejection.

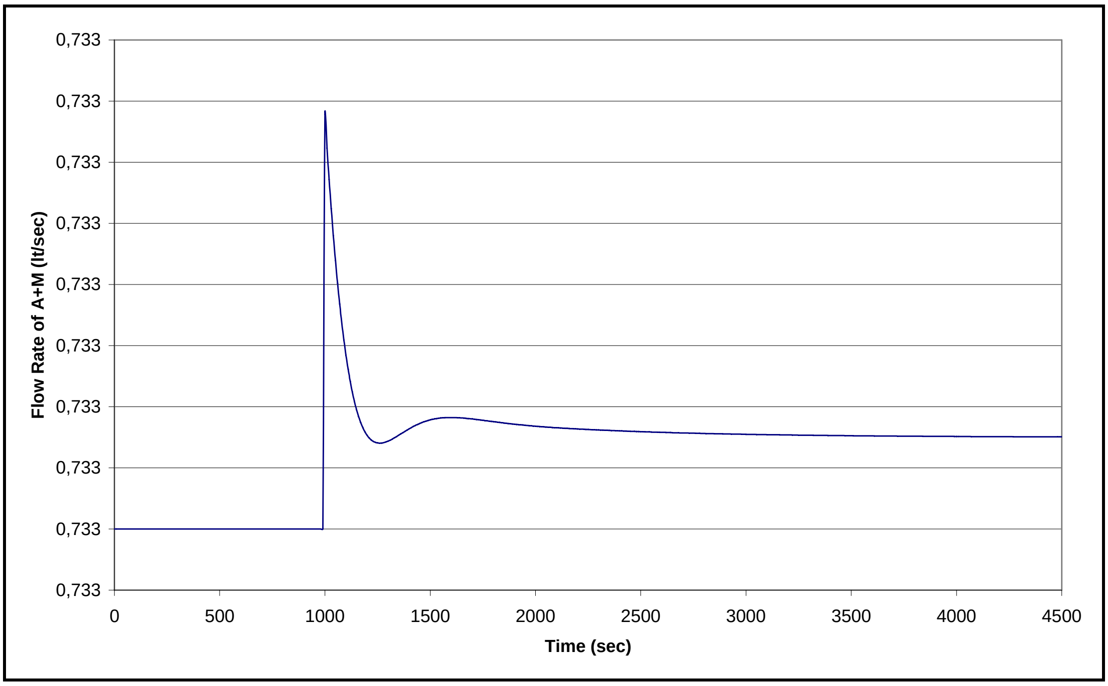


Figure 5.36 : Response of F_A to disturbance rejection.

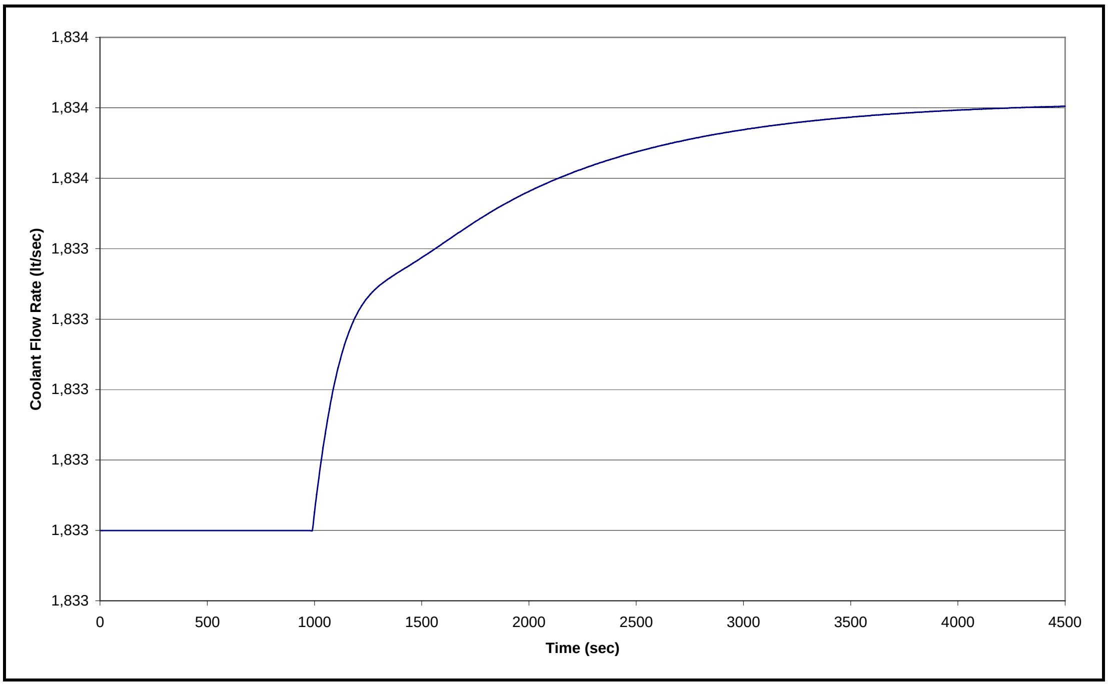


Figure 5.37 : Response of F_{CW} to disturbance rejection.

5.7 Comparison of MPC with PID control

After evaluating the MPC controller for set point tracking, disturbance rejection and robustness, a decentralized PID control is compared with the controller. Using general Ziegler-Nichols tuning rules, PID controller gain (K_C), integral time (τ_I) and derivative time (τ_D) are found as 25.2, 1.25 and 5 for the first loop and 258, 1.25, 5 for the second loop.

The performance of the controllers is evaluated by their set point tracking capability. Set point tracking problem discussed before is applied to PID. The results for response to propylene glycol concentration and reactor temperature are given in Figure 5.37. As can be seen from the Figure 5.38, MPC controller reaches the set point faster with smaller peak. IAE score also proves the fact with 13.632 for MPC and 18.98 for PID.

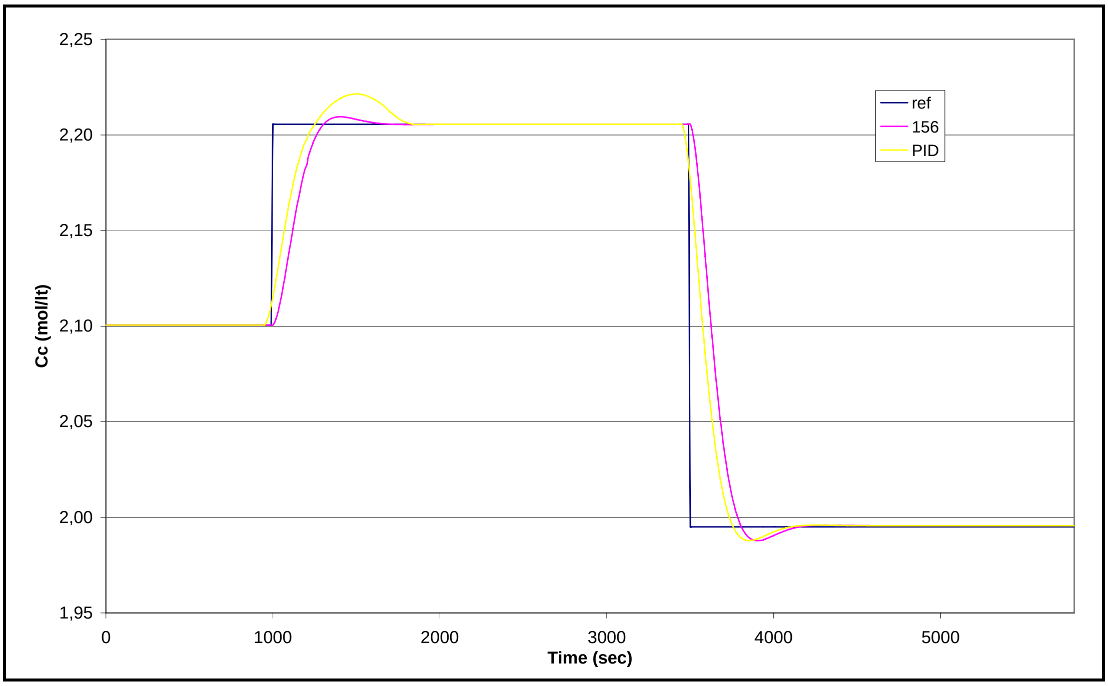


Figure 5.38 : Responses of PID and MPC controller of C_c for set point tracking.

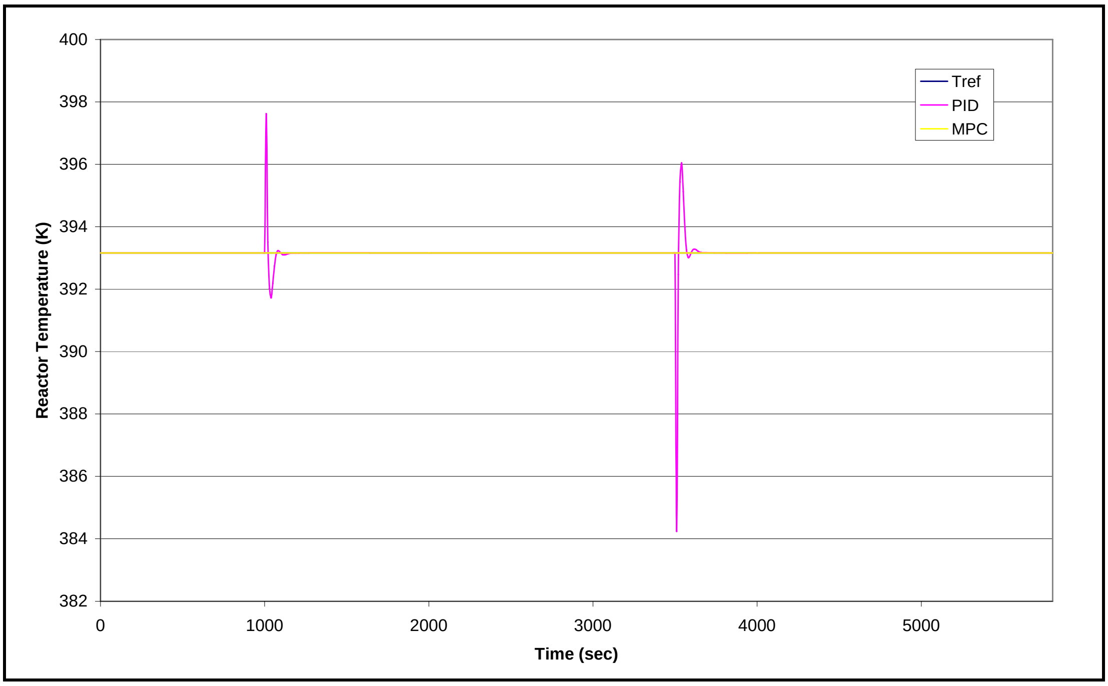


Figure 5.39 : Responses of PID and MPC controller of T for set point tracking.

6. CONCLUSION

In this study, control of a chemical engineering application, continuous stirred tank reactor, is to be examined by the use of Model Predictive Controller. As a case study, production of propylene glycol resulting from exothermic reaction of propylene oxide – methanol mixture with excess water with the acid catalyst is chosen.

The dynamic characteristics and interactions of the plant variables are investigated first. The model of the chemical reactor is obtained with mass and energy balances. Using balance equations, steady state values and steady state gain matrix are obtained. Analysis of steady state gain matrix by Singular Value Decomposition shows that the system is highly ill-conditioned and necessitates the use of a MIMO control algorithm. It was analyzed that, the control algorithm should have control the concentration of the product, propylene glycol, and the temperature of the reactor by manipulating propylene oxide – methanol mixture flow rate and coolant flow rate. Also initial concentration of propylene oxide and coolant temperature were considered as measured disturbances.

The controller algorithm was set up using the code derived in adaptation with MATLAB MPC toolbox, using the linear step responses. From possible tuning parameters Prediction Horizon, Control Horizon and the ratio of weighting vectors $f=\lambda_1/ \lambda_2$, Prediction Horizon was kept constant as 85 % of the Model Horizon. The tuning was carried out by starting with a fixed Control Horizon as 60 % of Model Horizon and altering f values to achieve a better set point tracking. For constant Prediction Horizon P = 221 and Control Horizon C = 156, different f values are evaluated. As a result the response of f = 0.01 was chosen as the most desired case. By changing Control Horizon at this value of f, the tuning is completed by defining the best response. The resulting controller had the weight ratio of f=0.01 and Control Horizon of C = 156.

The response of the controller was also tested for disturbance rejection. The system was disturbed by changes in the initial concentration of propylene oxide and coolant temperature. It was also seen that the controller did not degrade under disturbance presence.

Robustness of the controller was also tested by changing the system dynamic, a change in the reaction rate constant, and the system's response was examined. It was concluded that although some small deficiencies the controller responded well to the changes.

Finally the controller was compared with a traditional PID controller for set point tracking and MPC controller proved its superiority.

As future works, the realization of the reactor at laboratory level and the effect of modeling errors would be compared using real data. Also rather than step response model, more iterative methods would be used for prediction algorithm such as neural networks or fuzzy systems.

REFERENCES

[1] Afonso, P.A., Oliviera, N.M. and Castro, A.M., 1996.Model Predictive Control On A Pilot Plant Reactor With A Simulated Exothermic Reaction, *Computers & Chemical Engineering*, **20,** 769-774.

[2] Al-Ghazzawi,A. Ali, E., Nouh, A. and Zafiriou, E., 2001. Online Tuning Strategy For Model Predictive Controllers, *Journal of Process Control*, **11,** 263-284.

[3] Arkun, Y., 1978. Design of Steady-State Optimizing Control Structures For Chemical Processes. *Ph.D. Thesis*, University of Minnesota.

[4] Bemporad, A., Morari, M. and Ricker, N.L., 2006. Model Predictive Control Toolbox, Mathworks INC, New York.

[5] Biagiola, S.I. and Figueroa, J.L., 2004. Application of state estimations based NMPC to an unstable nonlinear process, *Chemical Engineering Science*, 59 4601-4612

[6] Camacho ,E.F. and Bordons,C., 1999. Model Predictive Control, Springer-Verlag Limited, London.

[7] Biegler, L., Cervantes, A.M. and Wachter, A., 2002. Advances In Simultaneous Strategies For Dynamic Process Optimization, *Chemical Engineering Science*, **57,** 575-593.

[8] Clarke, D.W., Mohtadi, C. and Tuffs, P.S., 1987. Generalized Predictive Control – Part I. The Basic Algorithm, *Automatica*, **23**, 137-148.

[9] Clarke, D.W., Mohtadi, C. and Tuffs, P.S., 1987. Generalized Predictive Control – Part II. Extensions and Interpretations, *Automatica*, **23,** 149-160.

[10] Cutler, C.R. and Ramaker, B.L., 1980. Dynamic Matrix Control-a Computer Control Algorithm, In proceedings of the joint automatic control conference, *National AIChE Meeting*

[11] Cutler, C.R. and Ramaker, B.L., 1980. Dynamic Matrix Control-a Computer Control Algorithm, *In proceedings of the joint automatic control conference*

[12] Fogler, H.S., 1999. Elements of Chemical Reaction Engineering, Prentice Hall International Series, New Jersey

[13] Garcia, G.E. and Morshedi, A.M., 1986. Quadratic Programming solution of Dynamic Matrix Control (QDMC), *Chemical Engineering Communications*, **46,** 73-87.

[14] Garcia,G.E., Prett,D.M. and Morari, M., 1989. Model Predictive Control:Theory and Practice – a Survey, *Automatica*, **25,** 335-348.

[15] Garcia, C.E. and Prett, D.M., 1989. Advances in industrial model predictive control, M.Morari and T.J. McAvoy (Eds), *Chemical Process Control* III, 249-294. CACHE and Elsevier, Amsterdam.

[16] Goodwin, G.C., Graebe, S.F. and Salgado, M.E., 2001. *Control System Design*, Englewood Clifffs, Prentice Hall, NJ.

[17] Grosdidier, P., Froisy, B. and Hammann, M., 1988. The IDCOM-M Controller, *in* T. J. McAvoy, Y. Arkun E. Zafiriou (eds), *Proceedings of the 1988 IFAC Workshop on Model Based Process Control*, 31-36.

[18] Hidalgo, P.M. and Brosilow,C.B., 1990, Nonlinear model predictive control of styrene polymerization at unstable operating points, *Computers & Chemical Engineering*, **14**, 481 – 489.

[19] Kassmann, D.E., Badgwell, T.A. and Hawkins, R.B., Robust Steady State Target Calculation for Model Predictive Controller, *AIChE Journal***, 46 (5),** 1007-1024.

[20] Kothare, M.V., Balakrishan, V. and Morari, M., Robust Constrained Model Predictive Control Using Linear Matrix Inequalities, *Automatica*, **32**, 1361-1379.

[21] Kwakernaak, H. and Sivan, R., 1972. Linear Optimal Control Systems, Wiley&Sons, New York.

[22] Lee, E.B. and Markus L., 1967. Foundations of Optimal Control Theory, Wiley & Sons, New York.

[23] Lee, J.H., Morari, M. and Garcia, C.E., 1994. State Space Interpretation of Model Predictive Controllers, *Automatica*, **30,** 707-717.

[24] Marquis, P. and Broustail, J.P., 1998. SMOC, A Bridge Between State Space and Model Predictive Controllers : Application to the Automation of a Hydrotreating Unit, In T. J. McAvoy, Y. Arkun,& E. Zafiriou (Eds.), Proceedings of the 1988 IFAC workshop on model based process control, 37-43.

[25] Marchetti, J.L., Mellichamp, D.A. and Seborg, D.E., 1983. Predictive Control Based on Discrete Convolution Models, *Ind. Eng. Chem. Process Des. Dev.*, **22,** 488-494.

[26] Martin, G.D., 1981. Long-Range Predictive Control, *AIChE Journal*, **27,** 748-753.,

[27] Moore, C., 1986**,** Application of Singular Value Decomposition to the Design, Analysis and Control of Industrial Processes, *ACC*, Seattle, 643-65

[28] Morari, M. and Lee, J.H., 1999. Model Predictive Control : Past, Present and Future, *Computers and Chemical Engineering*, **23,** 667-682.

[29] Muske, K.R. and Rawlings, J.B., 1993. Model Predictive Control with Linear Models, *AIChE Journal*, **39,** 262-287.

[30] Nagrath, D., Prosad, V. and Bequette, B.W., 2002. A Model Predictive Formulation for Control of an Open Loop Unstable Cascade Systems, *Chemical Engineering Science*, **57,** 365-378.

[31] Park, M.J. and Rhee, K., 2001. LMI Based Robust Model Predictive Controller for a Continuous MMA Polymerization Reactor, *Computers & Chemical Engineering*, **25,** 1513-1520.

[32] **Prasud, V., Schley, M., Russ, L. and Bequette, B.W.,** 2002. Product Property and Production Rate control of Styrene Polymerization, *Automatica*, **12,** 353-372.

[33] **Prett, D.M., and Garcia, C.E.,** 1988. Fundamental Process Control, Butterworth Publishers, New York.

[34] **Propoi, A.I.,** 1960. Use of Nonlinear Programming Methods for Synthesizing Sampled-data Automatic Systems, *Automatic Remote Control*, **24,** 837-844.

[35] **Qin, S.J. and Badgwell T.A.,** 2000. An Overview of Nonlinear Model Predictive Control Applications, Pr*ogress in Control and System Theory*, **26,** 369-392.

[36] **Qin, S.J. and Badgwell T.A.,** 2003. A survey of Industrial Model Predictive Control Technology, *Control Engineering Practice*, **11,** 733-764.

[37] **Richalet, J., Rault, A., Testud, J.L. and Papon,J.,** 1976. Algorithmic Control of industrial processes. In proceedings of the 4th IFAC symposium on identification and system parameter estimation, 1119-1167.

[38] **Richalet, J., Rault, A., Testud, J.L. and Papon,J.,** 1978. Model Predictive Heuristic Control:Application to Industrial Processes, *Automatica*, **14,** 413-428.

[39] **Riggs, J.B. and Rhinehart, R.R.,** 1990. Comparison between two nonlinear process-model based controllers, *Computers and Chemical Engineering*, **14,** 1075-1081.

[40] **Rouhani, R. and Mehra, R.K.,** 1982. Model Algorithmic Control (MAC). Basic Theoretical Properties, *Automatica*, **18,** 401-411

[41] **Santos, L.O., Afonso, P.A. and Castro, J.A.,** 2001. Online Implementation of Nonlinear Model Predictive Controller: an Experimental Case Study, *Control Engineering Practice*, **9,** 847-857.

[42] **Scokaert, P.O.M. and Mayne, D.Q.,** 1998. Min-max Feedback Model Predictive Control for Constrained Linear Systems, IEEE Transactions on Automatic Control, **43(8)**, 1136-1142.

[43] Seborg, D.E., Edgar, T.F. and Mellichamp, D.A., 1989. *Process Dynamics and Control*, John Wiley & Sons Inc., Canada.

[44] Sistu, P.B. and Bequette, B.W., 1992. A comparison of Nonlinear Control Techniques for Continuous Stirred Tank Reactors, *Chemical Engineering Science*, **47,** 2553-2558.

[45] Wu, F., 2001. LMI Based Robust Model Predictive Control and its Application to an Industrial CSTR Problem, *Journal of Process Control*, **11,** 649-659.

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