

MODELLING, SIMULATION AND DYNAMIC MATRIX CONTROL OF A METHANOL-TO-ETHENE PROCESS

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Abstract

This research has been carried out to develop a model for the methanol-to-ethene process, simulate it and carry out its dynamic matrix control by investigating the effects of some tuning parameters on the control system. In order to achieve this aim, the methanol-to-ethene (MTE) process was modelled and simulated with the aid of ChemCAD for both steady state and dynamics. The dynamics data showing the response of ethene mole fraction to a change in reflux ratio were extracted from the ChemCAD dynamic simulation of the developed process model and used to develop a first-order transfer function relation between ethene mole fraction and reflux ratio via the System Identification Toolbox of MATLAB. Furthermore, the open loop simulation of the process was carried out in MATLAB environment. Thereafter, the closed loop response of the system was obtained using different values of control horizon, prediction horizon, model length, and control weighting as the tuning parameters of the dynamic matrix controller while the set point of the process was made to be the achievement of a mole fraction of 0.95 for ethene. It was revealed from the results obtained that the ChemCAD and the transfer function models developed for the process were valid ones because the ethene mole fractions obtained at their steady states upon the application of a final value of 2 to the reflux ratio, which was the input variable of the process, were very close. Also, the simulations of the closed-loop system of the dynamic matrix control of the process showed that there were significant effects of the control horizon, prediction horizon, and control weighting on the dynamic matrix control of the methanol-to-ethene process whereas the effect of the model length was found to be insignificant. Therefore, it has been discovered that control horizon, prediction horizon, and control weighting were the main tuning parameters for the dynamic matrix control of the methanol-to-ethene process.

Keywords: Methanol; ethene; ChemCAD; dynamic matrix control; MATLAB; control horizon; prediction horizon; control weighting.

1. Introduction

To meet the ever-increasing demand for oil-based chemicals despite waning oil reserves, the development of new technologies from alternative feedstock is a general concern for both scientific and industrial communities [1]. One of the most prominent emerging technologies is the methanol-to-olefin (MTO) process that is catalyzed by acidic zeolites, such as H-ZSM-5, or by nanoporous zeotype materials, such as H-SAPO-34 [2].

Olefins can be produced using several processes and feedstocks. In every process, a range of products and byproducts are formed. The percentage of the different products depending on the process and the feedstock used. Currently, there are three main sources of olefins for petrochemicals, viz. steam cracking of hydrocarbons (naphtha, ethane, gas oil and liquefied petroleum gas), fluid catalytic cracking in oil refineries and paraffin dehydrogenation. In addition to these commercial processes, there are some non-commercial technologies under

various phases of development such as oxidative coupling of methane, oxidative dehydrogenation of paraffins and methanol-to-olefins process [3], which is being considered in this work.

According to the information from the research of Keil [4], the conversion of methanol to hydrocarbons, including methanol-to-olefin, was discovered by two teams of Mobil scientists working on unrelated projects. They discovered, by accident, the formation of hydrocarbons from methanol over the synthetic zeolite ZSM-5 in early 1970. The group at Mobil Chemical in Edison, New Jersey, had been trying to convert methanol to ethene oxide, while workers at Mobil Oil's Central Research Laboratory in Princeton were attempting to methylate isobutene with methanol in the presence of ZSM-5. Neither of the reactions yielded the expected result. Instead, aromatic hydrocarbons were formed.

The methanol-to-olefin process converts methanol into light olefins, such as ethene - an important feedstock for the production of many types of polymers, which serve as basic building blocks for petrochemical industries and polymerization processes in particular. As a result, ethene and propene are increasingly in demand [1] in process industries.

Recent interest in the methanol-to-olefin mechanism was further fueled by a surge in oil prices. methanol-to-olefin conversion allows the petrochemical industry to bypass crude oil as a fundamental feedstock because methanol can be made from synthesis gas, which, in turn, can be formed from almost any gasifiable carbonaceous species, such as natural gas, coal, biomass and organic waste [1]. This process has some advantages over the current steam cracking of natural gas liquids, naphtha or other light fractions of petroleum, due to the fact that methanol-to-olefin process can provide a wider and more flexible range of ethene to propene ratio relative to those of conventional processes to meet market demand [2].

For the purpose of this research work, the interest will be limited to the production of the simplest olefin, which is ethene. The methanol-to-ethene (MTE) process was got from the methanol-to-olefin process. The former was launched solely for ethene production. In both processes, methanol that is produced mainly from synthesis gas is used as the feed of the process [5].

Due to the fast development of the process industries, one of which is a methanol-to-ethene process, improving the plant efficiency is very challenging owing to the fact that the scale of processes has become larger and process complexity has increased dramatically. This has led to the demand of a very robust controller design strategy, both in theory and practice [2].

Based on that, Richalet [6] has classified the controllers for the control problems into four hierarchical levels:

1. first level controllers used for the control problems dealing with some ancillary systems, in which proportional-integral-derivative (PID) controller could be a very good choice,
2. the second level controller used for problems involving multivariable dynamic process, which is interfered by some unmeasured perturbations,
3. third level controllers used for optimization problems based on the minimization of cost functions; a model predictive controller (MPC) is in this level, and
4. fourth level controllers consisting of those time and space scheduling production problems that include the feasible research and have the best economic benefits.

As a result of the simple structure, low cost, convenient manipulation and the satisfaction for most of the production control, proportional-integral-derivative has become the major controller used in the family of level one. However, the economic benefits induced by level one and two are usually negligible [6].

The model predictive controller works in a different manner in the sense that instead of using the past error between the output of the system and the desired value like a proportional-integral-derivative controller would do, it controls the system by predicting the value of the output in a short time, so the system output is as closer as possible to its desired value for these moments. In process control today, more than 95% of the control loops are of proportional-integral-derivative type [7-8]. Also, it is stated that more than 90% of industrial controllers are still implemented based on proportional-integral-derivative algorithms [9]. However, the proportional-integral-derivative seems not to be robust and effective in some cases involving a methanol-to-olefin process.

Owing to that, it has been realized that there is the need to incorporate an advanced controller type such as the dynamic matrix control that is based on model predictive control technology to processes like the one of methanol-to-olefin type because it can bring about many improvements in the economics of the system, can easily deal with multivariable cases and can also be used to handle the process if there are delays. Therefore, the aim of this research work is to apply dynamic matrix control to a methanol-to-ethene process by taking the mole fraction of ethene obtained from the process and the reflux ratio as the controlled and the manipulated variables respectively.

2. Methodology

The methods adopted in accomplishing the control of the methanol-to-ethene (MTE) process are as outlined in the following subsections.

2.1. Steady State modeling and simulation of the MTE process

The process was modelled and simulated using ChemCAD [10] process simulator through the following steps:

- Component Selection:** The chemical components involved in the process were chosen from the ChemCAD database, and they were:
 - Methanol
 - Dimethyl ether
 - Ethene
 - Water
- Thermodynamic Package Selection:** Based on the components involved in the process, UNIQUAC Functional-group Activity Coefficients (UNIFAC) method was chosen as the thermodynamic package for the simulation.
- Flowsheet Development:** The different unit of the process flowsheet was selected from the Palette of the simulator and connected accordingly. The equilibrium reactor having one feed stream was connected to the kinetic reactor which was in turn connected to the Simultaneous Correction Distillation System (SCDS) column with two product streams, see Figure 1. The dehydration of methanol to dimethyl ether represented by Equation (1) was incorporated into the equilibrium reactor while the conversion of dimethyl ether to ethene and water, which is represented by Equation (2), was incorporated into the kinetics reactor using the kinetics expressions given in Equation (3) and (4) and the parameters contained in Table 5.
- Feed Stream Specification:** The conditions of the feed streams were specified as given in Table 1.
- Equipment Specification:** The conditions of the equilibrium reactor, kinetic reactor and SCDS column were specified using the operating parameters given in Tables 2 – 4 respectively.



Table 1. Operating parameters for feed stream

Parameter	Description/Value
Stream name	Methanol
Temperature (oC)	60
Pressure (atm)	1
Total flow (kmol/hr)	100
Methanol (mole fraction)	1

Table 2. Operating parameters of the equilibrium reactor

Parameter	Description/Value
Reactor type	General equilibrium reactor
Number of reactions	1
Thermal mode	Isothermal
Calculation mode	Approach delta T = 5 (°C)
Liquid Keq model	Keq = Kx

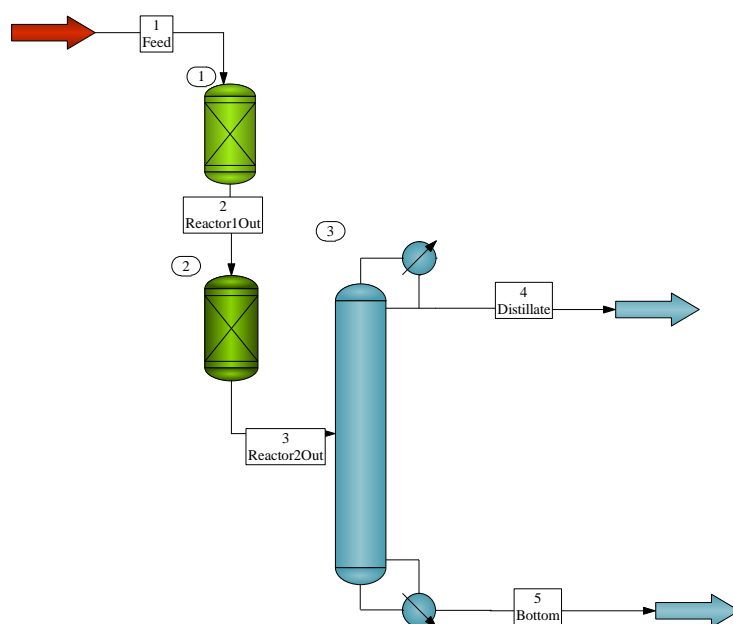


Figure 1. ChemCAD model of the methanol-to-ethene process

Table 3. Operating parameters of the kinetics reactor

Parameter	Description/Value
Reactor type	Plug flow
Number of reactions	1
Thermal mode	Adiabatic
Calculation mode	Volume specification and conversion calculation
Reactor volume	10 m ³

Table 4. Operating parameters of the SCDS column

Parameter	Description/Value
Condenser type	Total
Number of stages	11
Feed stage for column feed stream	5
Reflux ratio	1
Reboiler duty (kJ/sec)	0.1

The rate of reaction for the conversion of dimethyl ether to ethene is given as,

$$r = k_2 C_{DME} \quad (3)$$

where DME denotes dimethyl ether, and the rate constant is given as

$$k = k_0 e^{\frac{E}{RT}} \quad (4)$$

The kinetic data for modeling the reaction was obtained from the work of Jianglong and Huixin [11] as given in Table 5.

Table 5. Kinetics data for the conversion of dimethyl ether to ethane

Parameter	Value
k_0 (hr ⁻¹)	9.18×10^7
E (J/mol)	89478

Source: Jianglong and Huixin [11]

After developing the steady-state process model using ChemCAD, it was run using the 'Run All' icon on the ChemCAD flowsheet ribbon until convergence before converting it to the type used in the dynamic simulation.

2.2. Process dynamics simulation

The dynamic simulation of the methanol to ethene process was carried out using the following steps:

1. *Conversion of the steady-state model to dynamics type:* Using the developed converged steady state MTE model, the dynamics option was selected from the 'Steady state/Dynamics' drop-down menu found under "run" menu.
2. *Dynamics simulation:* The dynamic model was simulated at two run time steps:
 - First run time step: A time of 5 min with a 0.01 min interval was used, and the dynamic simulation was run from the initial steady state in this case.
 - Second run time step: A time of 1.5 hr with a 0.05 min interval was used for the second run time step from the current steady state. In this case, the reflux ratio of the column was changed to a final value of 2.
3. *Dynamics data extraction:* The dynamics data obtained were for the mole fraction of ethene in the column distillate stream (stream 4). The run time plot for the mole fraction of ethene in stream 4 was obtained using the 'Plot Dyn Streams' icon on the ChemCAD flowsheet ribbon. From the plot, the dynamic data were extracted to an excel worksheet by clicking the 'Data to Excel CSV file' option from the 'Chart' drop-down menu.

2.3. Process transfer function formulation

The process transfer function model used in this work was formulated by developing the relationship between ethene mole fraction (output variable) and reflux ratio (input variable) using the data generated from the developed ChemCAD model with the aid of the System Identification Toolbox of MATLAB [12] using codes written. By running the script, the dynamics data of the simulated MTE process was called from the Microsoft Excel Spreadsheet and exported to the System Identification Toolbox interface of the MATLAB. On the System Identification Toolbox interface, a transfer function model of the form shown in Equation 5 was specified and developed.

$$G_p(s) = \frac{K_p e^{-T_d s}}{(1 + T_p s)} \quad (5)$$

2.4. Dynamic Matrix Control of the MTE Process

2.4.1. Formulation of control objective function

The dynamic matrix control (DMC) of the methanol-to-ethene process was accomplished using the method described by Bequette [13] in which the least-squares objective function for a control horizon of nc and a prediction horizon of np was as defined in Equation (6),

$$\Phi = \sum_{i=1}^{np} (y_{sp} - \hat{y}_{k+i})^2 + w \sum_{i=0}^{nc-1} (\Delta u_{k+i})^2 \quad (6)$$

where y_{sp} is the setpoint, \hat{y}_{k+i} is the model prediction at time $k+i$, w is the control weighting and u_{k+i} is the manipulated input at time step $k+i$.

The method was, actually, based on step response model that has the form given in Equation (7),

$$\hat{y}_k = \sum_{i=1}^{N-1} s_i \Delta u_{k-i} + s_N u_{k-N} \quad (7)$$

where \hat{y}_k is the model prediction at time step k , s_i represents the step response coefficient for the i th sample after the unit step input change, u_{k-i} is the manipulated input i steps in the past and u_{k-N} is the manipulated input N steps in the past.

As such, the control objective function was written as given in Equation (8),

$$\Phi = (E - S_f \Delta u_f)^T (E - S_f \Delta u_f) + (\Delta u_f)^T W \Delta u_f \quad (8)$$

where E is the unforced error vector,

$$S_f = \begin{bmatrix} s_1 & 0 & 0 & \cdots & 0 & 0 \\ s_2 & s_1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & & & & \\ s_j & s_{j-1} & s_{j-2} & \cdots & \cdots & s_{j-M+1} \\ \vdots & \vdots & \vdots & & & \vdots \\ s_P & s_{P-1} & s_{P-2} & \cdots & \cdots & s_{P-M+1} \end{bmatrix} \quad (9)$$

$$\Delta u_f = \begin{bmatrix} \Delta u_k \\ \Delta u_{k+1} \\ \vdots \\ \Delta u_{k+M-2} \\ \Delta u_{k+M-1} \end{bmatrix} \quad (10)$$

and

$$W = \begin{bmatrix} w & 0 & 0 & 0 \\ 0 & w & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & w \end{bmatrix} \quad (11)$$

The solution of the objective function was thus, also, carried out in MATLAB environment.

2.4.2. Tuning and simulation of the control system

The tuning parameters (control horizon, prediction horizon, model length, and control weighting) of the dynamic matrix control system were varied, and their effects on the control performance were investigated with the aid of MATLAB *mfile* codes written. It should be noted that, before tuning and controlling the system, the first-order-plus-delay-time transfer function of the system was approximated to an ordinary first order system using Pade approximation in order to convert the model to the form required by the approach of Bequette [13], which was the one adopted in this work.

3. Results and discussion

3.1. ChemCAD Steady-State simulation output

The results obtained from the steady-state simulation of the developed ChemCAD process model of the methanol-to-ethene (MTE) process were as given in Tables 6. Based on the information given in the table, the production of ethene using the process was a successful one because the mole fraction of ethene obtained was approximately 0.73 while the other main component present in the product was water with a mole fraction of approximately 0.25. The mole fractions of the other chemicals (methanol and dimethyl ether) involved in the process were found to be negligible. Based on the results of the steady-state simulation of the process, it was observed that a high concentration of the main product (ethene) could be obtained.

Table 6. Steady-state product stream component mole fraction

Component	Mole fraction
Methanol	0.01925
Dimethyl Ether	6.7166e-08
Ethene	0.7318
Water	0.2489

3.2 ChemCAD dynamic simulation output

Having ensured that the developed ChemCAD model of the process converged under steady state, it was converted to a dynamic type and simulated accordingly. The results of the dynamic simulation of the process are given in Figure 2 when a step change was applied to the reflux ratio, which was the input variable of the process, to make its final value to be 2.

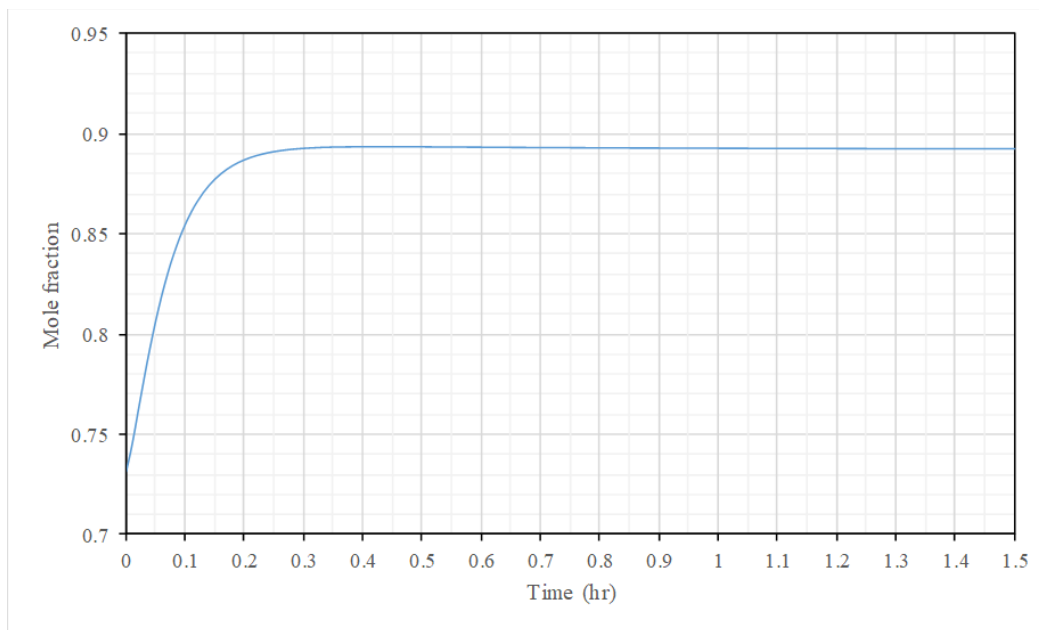


Figure 2. Dynamic response of the system in terms of the mole fraction of ethene mole fraction against time

It can be seen from Figure 2 that ethene mole fraction was affected by the change in the reflux ratio because it (ethene mole fraction) was found to vary from its initial steady state value of 0.7318 to another final steady state of approximately 0.8920. Therefore, it can be said that a change in the column reflux ratio has caused a change in the dynamic response of ethene mole fraction. In other words, the reflux ratio was an appropriate input variable for the process.

3.3. Transfer function modelling and Open-Loop simulation response

A first order transfer function with time delay was developed with the aid of System Identification Toolbox of MATLAB Using the data generated from the dynamic simulation of the process. The developed transfer function relating the ethene mole fraction (output variable) to the reflux ratio (input variable) in Laplace transforms was as given in Equation (12).

$$x(s) = \frac{0.44738}{7.3869s+1} e^{-0.25s} R(s) \quad (12)$$

The open-loop simulation of the developed transfer function model of the process was also carried with the aid of MATLAB *mfile* by applying a step change with a final value of 2 to the reflux ratio, and the dynamic response obtained is given in Figure 3.

From the open loop response shown in Figure 3, it was again confirmed that the system was a stable one as it could attain an ethene steady-state value of approximately 0.8942 within 50 min of the simulation period. This steady-state value was found to be in agreement with the one obtained from the ChemCAD dynamic simulation of the process. Though the system was found to be a stable one, in order to obtain an ethene mole fraction higher than the one obtained from the open-loop steady-state simulation, there was the need for its proper control using an advanced control method known as dynamic matrix control.

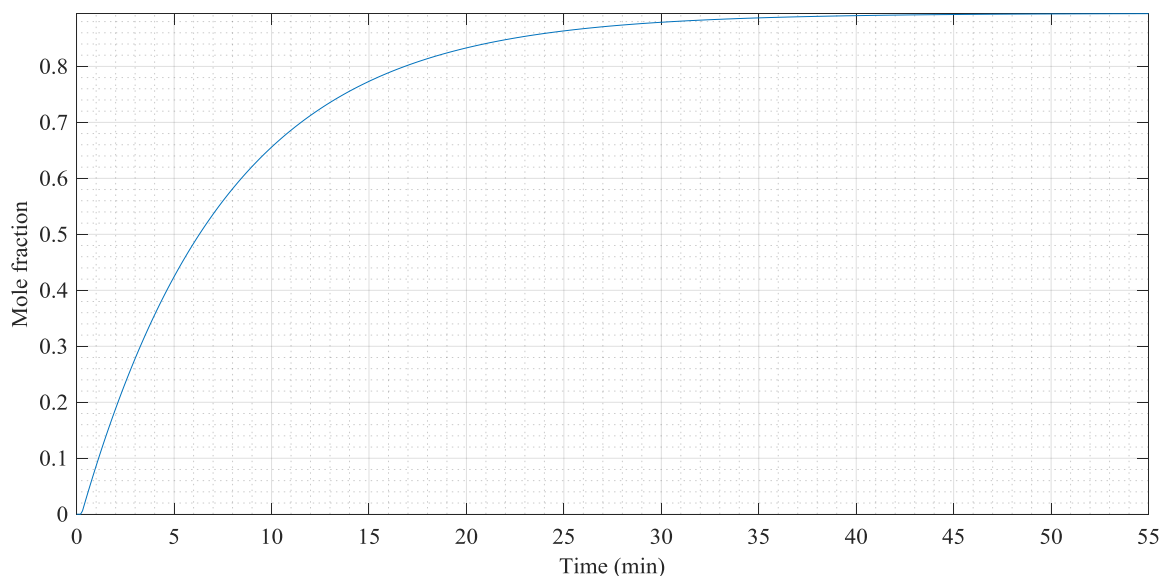


Figure 3. Open loop response of the process to a unit step change in reflux ratio

3.4. Dynamic matrix control simulation

The dynamic matrix control of the methanol-to-ethene process was carried out by investigating the effects of the tuning parameters (control horizon, prediction horizon, model length, and control weighting) on the performance of the system towards giving ethene mole fraction of 0.95 as the controlled variable while the reflux ratio was taken as the manipulated variable.

3.4.1. Effect of control horizon

Control horizon refers to the sequence of control moves required to satisfy the specified optimization objective of minimizing the predicted deviation of the process output from the target over the prediction horizon and the expenditure of control effort in driving the process output to the target in the presence of prespecified operating constraints. Since this variable is used in the optimization of the control function, it means it is very important to the performance of the control system. As such, it is worth investigating how it affects the dynamic matrix control of the methanol-to-ethene process. The results of the investigation carried out by making the value of the control horizon to be 1 and 5 are given in Figure 4. According to the results given in the figure, the response of the control system was found not to have any overshoot when the control horizon was 1 whereas that of the control horizon of 5 had overshoot. However, the response of the control horizon of 5 was observed to get settled faster than that of the control horizon of 1.

Table 7. Performance criteria values for effects of control horizon

Criterion	Control horizon = 1	Control horizon = 5
SAE	7.3294	5.8830
MAE	0.1018	0.0817
SSE	4.3084	4.1008
MSE	0.0598	0.0570

In order to further know the effect of the control horizon on the performance of the control system, some performance criteria, which were sum of absolute error (SAE), mean of absolute error (MAE), sum of squared error (SSE) and mean of squared error (MSE), were calculated for the two cases considered in this work, and the results obtained are given in Table 7. The values of the criteria given in the table revealed that the performance of the control system when the control horizon was 5 was better than that of the control horizon of 1 because all

the values of the performance criteria of the control horizon of 5 were less than those of the control horizon of 1, keeping other tuning parameters constant.

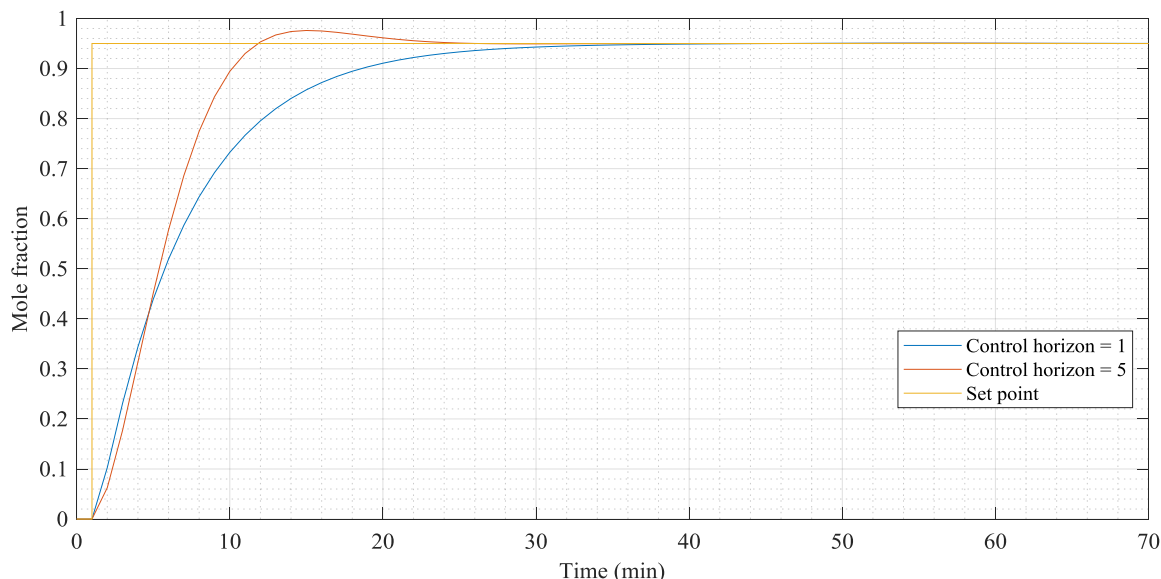


Figure 4. Closed-loop response of the MTE process to a step change of 0.95 in ethene mole fraction and variation in control horizon; prediction horizon = 25, model length = 50, control weighting = 0.3

3.4.2. Effect of the prediction horizon

The prediction horizon is the number of a prediction made on the process over a predetermined time horizon beyond the extent of the control action, and it is another tuning parameter that affects the response obtained from the dynamic matrix control system. The investigation of its effect on the dynamic matrix control of the methanol-to-ethene process was carried out by varying its value from 15 to 35, and the responses obtained were as given in Figure 5. The responses in the figure showed that the variation in the closed-loop dynamic response of the process was not much despite the 20-unit difference in the values of the prediction horizon, as compared to the response obtained when the control horizon was changed from 1 to 5. This is to say that the response of the dynamic matrix control of this process was more sensitive to the control horizon than to the prediction horizon.

In an attempt to know how the change in the prediction horizon was affecting the control system involving the methanol-to-ethene process, the selected performance criteria were also calculated in this case, and the results are given in Table 8. The closeness of the performances of the control systems with prediction horizons of 15 and 35 could also be seen from the performance criteria results because the values of SAE, MAE, SSE and MSE for the two cases considered were found to be close for each criterion.

Table 8. Performance criteria values for effects of prediction horizon

Criterion	Prediction horizon = 15	Prediction horizon = 35
SAE	6.1494	6.3923
MAE	0.0854	0.0888
SSE	4.2396	4.3601
MSE	0.0589	0.0606

Moreover, however, the importance of the prediction horizon was shown clearly by comparing the responses in Figures 4 and 5 because it was clearly observed that the responses obtained when the prediction horizon was varied could get settled faster than those obtained when the control horizon was varied.

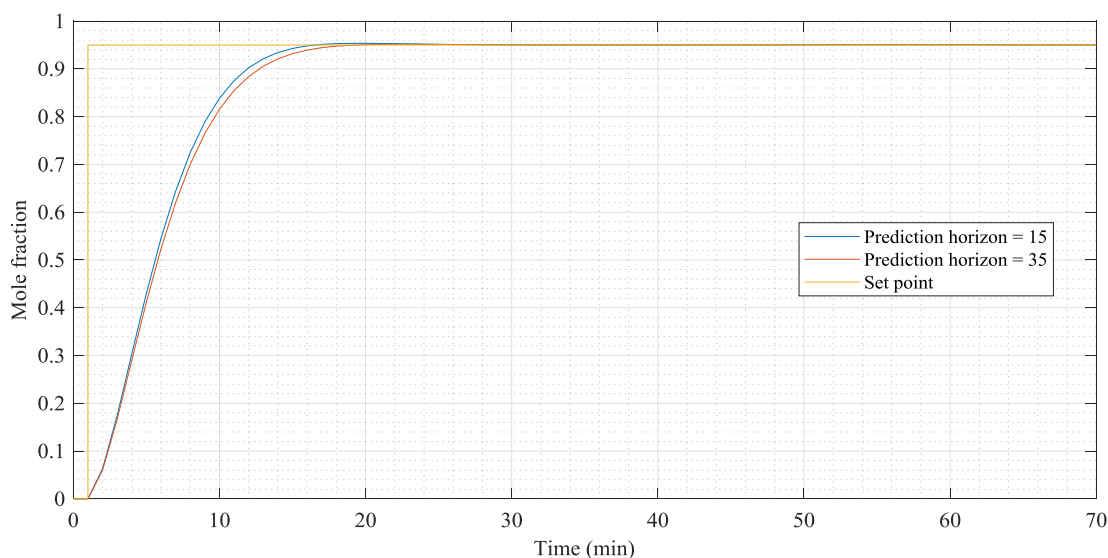


Figure 5. Closed-loop response of the MTE process to a step change of 0.95 in ethene mole fraction and variation in prediction horizon; control horizon = 3, model length = 50, control weighting = 0.3

3.4.3. Effect of model length

Another parameter affecting the responses obtained from dynamic matrix control is the model length. The model length of a dynamic matrix control should be selected in such a way that it is approximately the time required for the system to get to a new steady state. According to the information obtained from the literature, the model length for most systems is approximately 50 coefficients. That value of 50 was taken as the middle value in this work, and the simulation of the control system was carried out using a model length of 35 and 65 successively, and the results obtained are given in Figure 6. From the figure, it could be observed that the two responses obtained overlapped each other almost throughout the simulation time used for the dynamics. This is showing that the effect of model length chosen for the dynamic matrix control of this process is not significant.

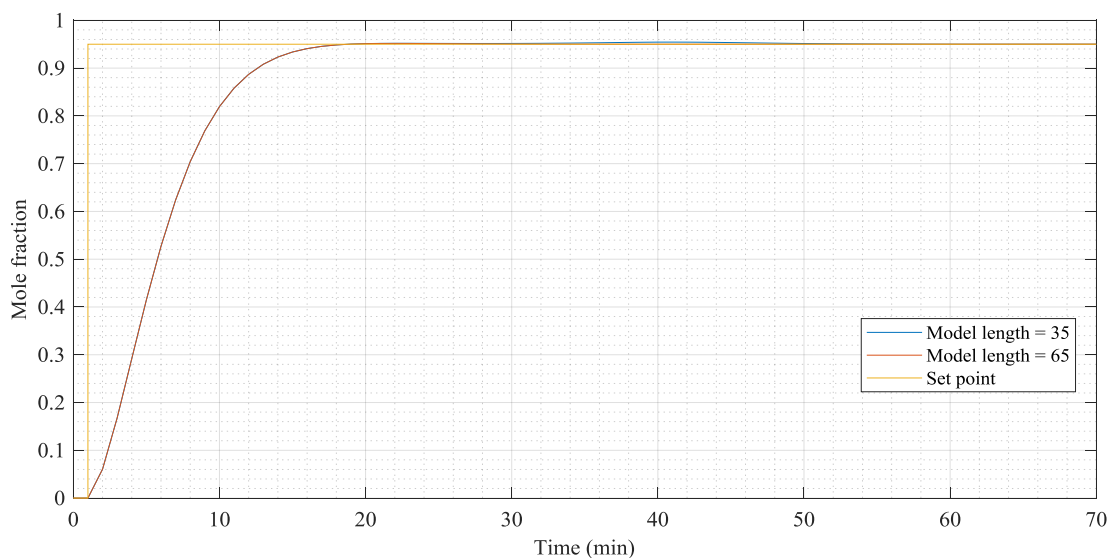


Figure 6. Closed-loop response of the MTE process to a step change of 0.95 in ethene mole fraction and variation in model length; control horizon = 3, prediction horizon = 25, control weighting = 0.3

Table 9. Performance criteria values for effects of model length

Criterion	Prediction horizon = 35	Prediction horizon = 65
SAE	6.4119	6.3408
MAE	0.0891	0.0881
SSE	4.3393	4.3391
MSE	0.0603	0.0603

This argument was also found to be supported by the values of the performance criteria that were calculated to be very close to each other for each criterion (see Table 9).

3.4.4. Effect of control weighting

Another parameter used in tuning the dynamic matrix control for this methanol-to-olefin process was the weighting factor. In this case, it was varied from 0.1 to 0.5 and the results obtained were as given in Figure 7.

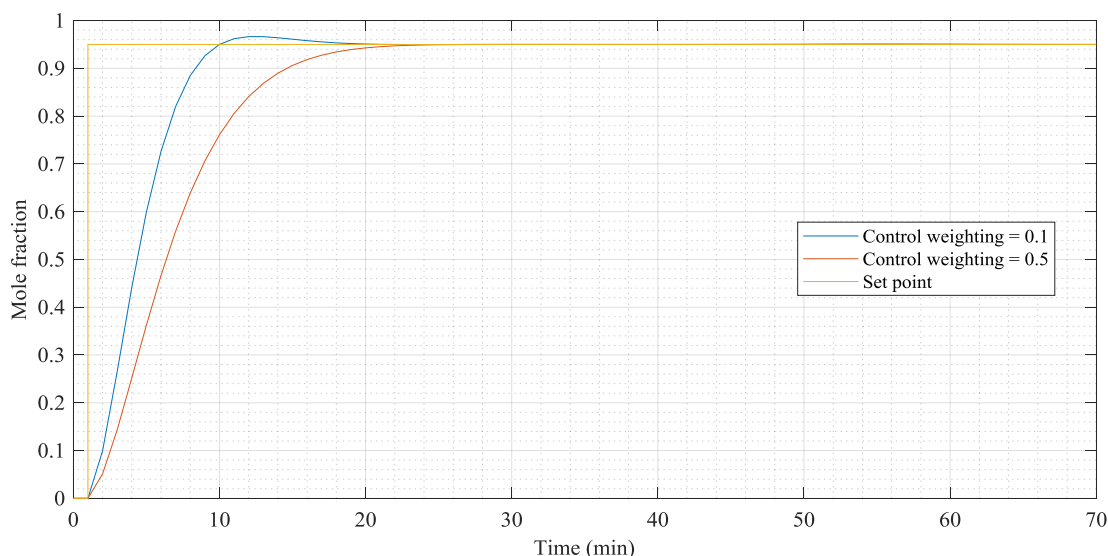


Figure 7. Closed-loop response of the MTE process to a step change of 0.95 in ethene mole fraction and variation in control weighting; control horizon = 3, prediction horizon = 25, model length = 50

Table 10. Performance criteria values for effects of control weighting

Criterion	Control weighting = 0.1	Control weighting = 0.5
SAE	4.8363	7.0623
MAE	0.0672	0.0981
SSE	3.4539	4.7237
MSE	0.0480	0.0656

From the results shown in Figure 7, it was clear that there is a dependency of the performance of dynamic matrix control on the control weighting because there was a clear difference between the two responses obtained when the values of the weighting factor were made to be 0.1 and 0.5.

The criteria values calculated for the variation of the control weighting showed that the performance of the dynamic matrix control was better when the control weighting was 0.1 than when it was 0.5 because all the performance criteria values of control weighting of 0.1 were less than those of the control weighting of 0.5.

4. Conclusion

The results obtained from the simulations carried out on the ChemCAD and the transfer function process models developed for the methanol-to-ethene production showed that the

models were valid ones because the steady-state values of ethene mole fraction given by the two models when the final value of the reflux ratio, which was the input variable, was 2 were very close. Furthermore, the closed-loop simulations of the dynamic matrix control system formulated for the process for investigating the effects of some tuning parameters (control horizon, prediction horizon, model length and control weighting) revealed that the control horizon, prediction horizon, and control weighting showed significant effects on the performance of the control system while the effect of the model length was found not to be significant for the methanol-to-ethene process. In addition, in all the cases, the process was observed to get settled within 45 min. Therefore, it can be inferred that the dynamic matrix control exhibited good control ability on the methanol-to-ethene process considered in this work.

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