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Polymerization Reactor Control under Uncertainty

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Table of Contents

List of Tables

List of Figures

Abstract

The need to control uncertainty has existed since the dawn of industrial chemical processes. Improper handling of uncertainty can lead to unsatisfactory product quality, profit losses, and safety issues. Generally, there are two ways to deal with uncertainty: overdesign and control. Controllers can be added to minimize the affects of uncertainty and keep the system from instability. This case study considers the design and control of a polymerization reactor with azo-*bis*-isobutyronitrile (AIBN) as the initiator, toluene as the solvent, and methyl methacrylate (MMA) as the monomer under uncertainty.

While a steady-state model is useful to understand a small part of the process, a dynamic model is needed to make a realistic assessment of what factors will drive the system out of the desired range. In order to compare the adverse affects of uncertainty, four control actions were implemented: proportional controller (P-controller), proportional-integral controller (PI-controller), Internal Model Control (IMC), and Model Predictive Control (MPC). From control models, it was possible to determine which uncertain parameters had greater effect on the product quality. The effects of uncertainty can be minimized by applying one or more optimally tuned control schemes. With an open-loop response of the system, optimal tunings can be found using tuning rules. After evaluating each controller, a quantitative method for comparison was needed, so cost models were applied to each controller. Despite the having the greatest capital investment, MPC minimized total costs far greater than the other control schemes. Four different design decisions (volume of the reactor) were also considered. Using a cost comparison, it was clear that simultaneously optimizing design and control decisions for given process parameters was not only possible but applicable. Model sensitivity can be determined for an optimally controlled process by finding the situation in which uncertainty will most adversely affect the

system. Sensitivity testing allows for greater prediction if, on an individual process basis, uncertain variables should be handled with control and with what magnitude that control should be applied.

Introduction

Control and Uncertainty

In chemical processes, there are generally two methods to deal with uncertainty: overdesign and control. The first method, overdesign, can be represented quantitatively as a safety factor. Overdesign is used to prepare the process for uncertainty so the product remains at a satisfactory level[1]. The second method, control, attempts to minimize the effect of uncertainty by predicting or measuring the uncertainty and attempting to adjust the system to it. These methods include feedback, feed-forward, and cascade control schemes. The classical design method begins with the process engineers designing the best process flow sheet while keeping capital and operating costs at a minimum. This flow sheet, along with all process parameters, is then given to the control engineers that design the best control scheme for the given process[1]. To best know how to handle uncertainty, either with design or control, a full understanding of the actual chemical reactions occurring is of great importance. Since both methods work towards the same goal of minimization of the affects of uncertainty, it would be beneficial if they could be combined into one optimization problem instead of being optimized separately.

Uncertainty exists in three forms: property, operational, and model. Property uncertainty comes from being unable to exactly know the chemical properties of a substance (density, molecular weight, etc). Operational uncertainty arises from uncontrollable factors affecting the chemical process. An example would be a pump that, nominally, pumps 100 liters per minute but could actually be pumping somewhere between 95 to 105 liters per minute at any given time. Model uncertainty arises from assumptions about the system that are not completely valid, such as, assuming a chemical process has a certain vapor-liquid equilibrium point when it is actually slightly different. This uncertainty can be quantitatively shown as the difference between the

nominal value of the variable and the extremes between which it could fluctuate. Uncertainty analysis is of great importance for many reasons. The effects of uncertainty can greatly affect the efficiency, safety, or even operability of chemical process. Typically, these fluctuations in operating conditions create shifts in the chemical process dynamics which ultimately lead to diminished quality of the product. In extreme cases, unhandled uncertainty could create unsafe conditions for operating. A logical and accurate way to deal with uncertainty while also obtaining optimal products is needed. This case study considers the design and control of a polymerization reactor with azo-*bis*-isobutyronitrile (AIBN) as the initiator, toluene as the solvent, and methyl methacrylate (MMA) as the monomer under uncertainty.

Polymerization

This work considers a polymerization reactor that utilizes free-radical polymerization. Free-radical polymerization occurs in three stages: initiation, propagation, and termination. Since monomers will not enter free-radical form by themselves, due to it being a greatly unstable form, an initiator is needed to begin the chain-reaction[4].

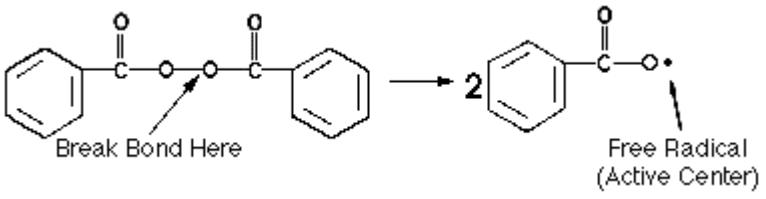

Figure 1 – Formation of polymers: the initiation reaction

The initiator begins the reaction by splitting into two free-radicals in the presence of the monomer. The highly-unstable free-radical must find another electron to form a stable bond. This need creates the next stage called propagation.

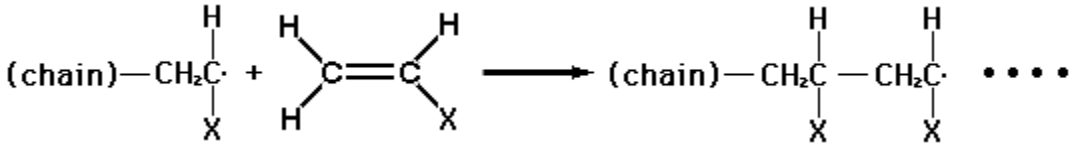

Figure 2 – Formation of polymers: the propagation reaction

The free-radical on the initiator reacts with one of the carbons on the end of the monomer by breaking the double bond. This leaves the last carbon of the monomer with a free-radical that will undergo the same process with another nearby monomer. This chain reaction occurs until it reaches a step known as termination. Termination has two avenues to pursue.

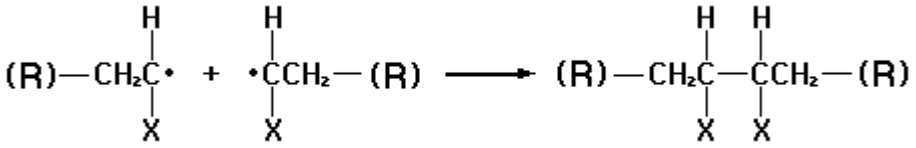

Figure 3 – Formation of polymers: the termination reaction - combination

The first method of termination is called combination. Combination involves two forming free-radical chains combining to create a sigma bond and forming the final polymer.

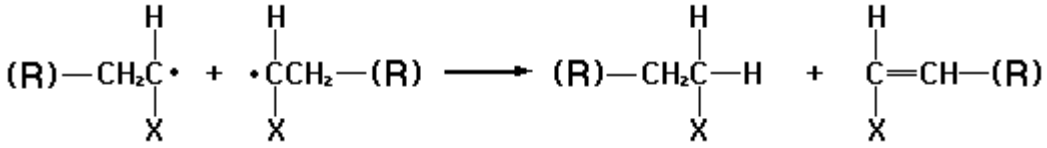

Figure 4 – Formation of polymers: the termination reaction – disproportionation

The second method of termination is called disproportionation. This occurs by the free-radical of one growing chain removing a hydrogen atom from the neighboring carbon of another free-radical chain. This ends the reaction by neutralizing all free-radicals.

Methodology

Models

An accurate and easily manipulated model is needed to show how the process will operate under changing conditions. This was accomplished by using Matlab[5] to solve the non-linear and differential equations. By programming the equations and parameters into Matlab, it was easy to change many parameters and see the effect quickly. Since in the steady-state model the accumulation term is zero, the non-linear solver "fsolve" was used. Dynamic models were also made for the non-isothermal case by implementing a step change in three variables to simulate uncertainty. Solving the differential equations required use of the "ode15s" solver in Matlab. After allowing the dynamic models to reach a new steady-state, controls were added to return to the process back to the desired steady-state.

Controllers

All controllers used in this work were feedback controllers. A feedback controller operates by detecting an output variable of a process and sending it to a controller. The controller then makes a control decision on how to best correct any deviation seen in the sensor from the set point value. Another signal is then sent to an actuator which changes the process dynamics through changing a manipulated variable. This process can be seen in .

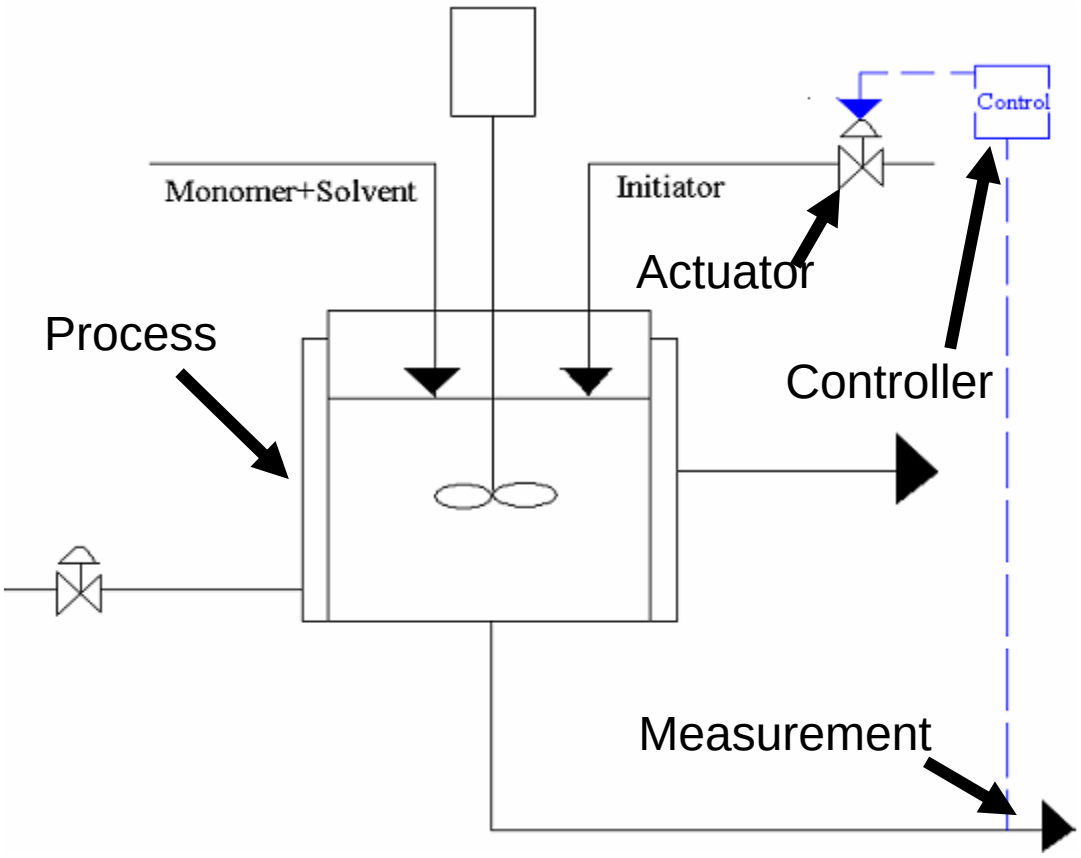

Figure 5 - Feedback control loop

The first control scheme implemented was a proportional controller (P-controller), equation (1),

$$C_f = K_c \cdot \varepsilon(t) + C_n \qquad (1)$$

where C_f is the actual output of the control variable, K_c is the gain of the system (constant value), $\varepsilon(t)$ is the error between the desired measured variable and the actual measured variable, and C_n is the nominal input of the controlled variable when the error is zero. The gain was incrementally changed until an acceptable model response was observed. That gain was considered to be an approximate optimal gain.

The second controller added was a proportional-integral controller (PI-controller), equation (2),

$$P(t) = K_c \cdot \left(\varepsilon(t) + \frac{1}{\tau} \int_0^t \varepsilon(t) dt \right) + P_s \tag{2}$$

where τ is the lag time. Since it is not possible to put the integral action of the controller in the code, the integral was changed to the equivalent form, equation (3),

$$\frac{dI}{dt} = \varepsilon(t) \tag{3}$$

evaluated as a seventh differential equation, and put into Matlab code as equation (4).

$$C_f(t) = K_c \cdot \left(\varepsilon(t) + \frac{1}{\tau} I \right) + C_n \tag{4}$$

The optimal gain and lag time could be approximated by making systematic changes in them until an acceptable response was seen.

Optimal Tuning

Using Ziegler-Nichols Approximate Model PID Tuning Rules[6], Table 1, and Cohen-Coon Approximate Model PID Tuning Rules[6], Table 2, it was possible to verify that the approximate optimal gains found earlier were reasonably close to those suggested by Ziegler-Nichols and Cohen-Coon. These tuning parameters will only apply to the P and PI controller since the other controllers have different methods of finding optimal tuning. The parameters τ, α, and K were taken from an open-loop response, for example, as in Figure 6.

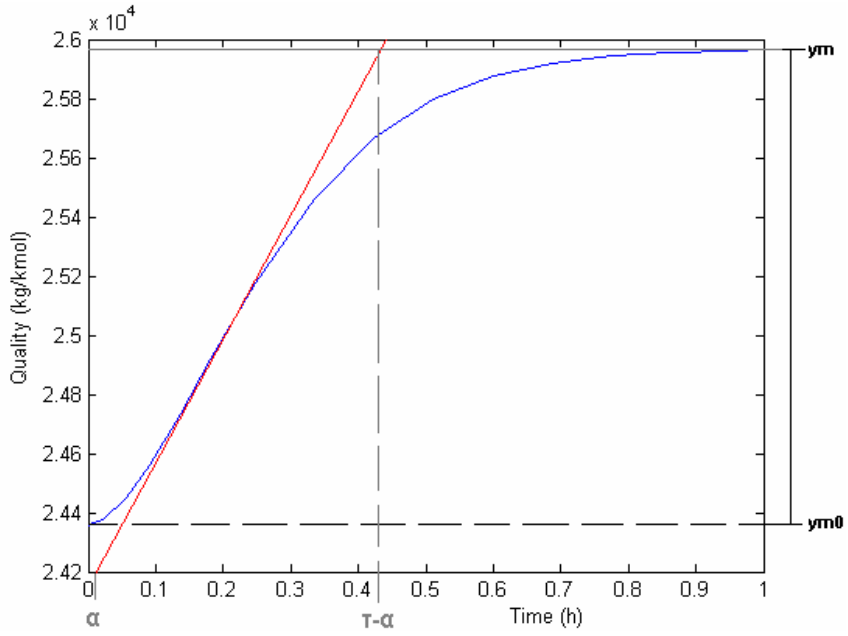

Figure 6 - Open loop response for non-isothermal dynamic model with uncertainty (U_{step}=0.99*U, cmi_{step}=0.985*cmi, and Tin_{step}=0.999*Tin)

K is obtained from the relationship in equation (5),

$$K = \frac{ym - ym0}{|SC|} \tag{5}$$

where SC is the magnitude of the step change.

Table 1 – Ziegler Nichols Approximate Model Tuning Rules

Controller Type	K_c	τ
P	$\frac{1}{K}\cdot\left(\frac{\tau}{\alpha}\right)$	-
PI	$\frac{0.9}{K}\cdot\left(\frac{\tau}{\alpha}\right)$	3.33α

Table 2 - Cohen-Coon Approximate Model Tuning Rules

Controller Type	K_c	τ
P	$\frac{1}{K}\cdot\left(\frac{\tau}{\alpha}\right)\cdot\left[1+\frac{1}{3}\cdot\left(\frac{\alpha}{\tau}\right)\right]$	-
PI	$\frac{1}{K}\cdot\left(\frac{\tau}{\alpha}\right)\cdot\left[0.9+\frac{1}{12}\cdot\left(\frac{\alpha}{\tau}\right)\right]$	$\alpha\left[\frac{30+3\cdot\left(\frac{\alpha}{\tau}\right)}{9+20\cdot\left(\frac{\alpha}{\tau}\right)}\right]$

These tuning tables were applied to the non-isothermal P-controller and PI-controller cases.

IMC Controller

The third controller implemented was IMC, or Internal Model Control. The IMC system was derived by taking parameters from the open loop response and applying IMC conversion, as in Figure 6. Since α was very small, it was considered to be zero for this controller. The transfer function of the process, g(s), was defined as in equation (6).

$$E_{i_j}\ g(s)=\frac{K_c}{\tau s+1} \tag{6}$$

Since this function, g(s), can be inverted due to it's lake of an exponential term we may know use equation (7),

$$c(s)=\frac{1}{g(s)}\cdot f(s) \tag{7}$$

where f(s) is defined as in equation (8).

$$f(s)=\frac{1}{(\lambda s+1)^n} \tag{8}$$

The parameter, λ, is the single tuning parameter for the IMC controller and n is chosen to be 1. c(s) is then passed into the conventional relationship between feedback controllers, $g_c(s)$ and IMC controller, c(s), as in equation (9),

$$g_c(s) = \frac{c(s)}{1 - c(s) \cdot g_I(s)} \tag{9}$$

where $g_I(s)$ is given as the case where both g(s) and the disturbance are known, or a "perfect" model of g(s). We then assume that $g_I(s)$ is very close to the "perfect" model of g(s), so that equation (10) applies.

$$g_I(s) = g(s) \tag{10}$$

The feedback controller transfer function then becomes equation (11).

$$g_c(s) = \frac{\tau}{K\lambda}\left(1 + \frac{1}{\tau s}\right) \tag{11}$$

This is the equivalent form of a PI controller in Laplace domain. By using this translation, we obtain a single "one knob" tuning parameter, λ, with the gain defined in equation (12),

$$K_c = \frac{\tau}{K\lambda} \tag{12}$$

and the now constant lag time, τ_I, defined as in equation (13)[6].

$$\tau_I = \tau \tag{13}$$

MPC Controller

The last controller implemented was MPC, or Model Predictive Control. MPC works by predicting possible trajectories that the process could take when under uncertainty. The best control trajectory is then obtained by solving an optimization problem at each time and implementing only the next control move. The entire process is repeated at each chosen time. Since this control scheme is very rigorous, it is commonly thought of as the closest thing to "perfect control" that is available. MPC is also very strong in that it can optimize the movement of many different manipulated variables at once where the classical controls (P, PI) and IMC cannot. The MPC model in MATLAB was provided from earlier work[11].

Cost Model Approximation

In order to determine which controller was economically profitable, a cost model needed to be assembled for each controller. The cost model was implemented as in equation (14).

$$Cost_t = Cost_{Cap} + Cost_{Op} - profit \tag{14}$$

The capital costs, equation (15), consisted of the reactor price, equation (16), the heat exchanger price, equation , and the controller price, Table 3.

$$Cost_{Cap} = Cost_r + Cost_{HE} + Cost_{Control} \tag{15}$$

$$C_r = C_{r,BC} \cdot \left(\frac{V_r}{V_{r,BC}} \right)^{0.63} \tag{16}$$

$$C_{HE} = C_{HE,BC} \cdot \left(\frac{A}{A_{BC}} \right)^{0.65} \tag{17}$$

Table 3 - Estimated controller prices

Controller	Estimated Price (USD)
P-Controller	$500
PI-Controller	$1,000
IMC	$2,000
MPC(PC Based)	$5,000
MPC(DCS Based)	$80,000 - $100,000

Reactor and heat exchanger correlation data was found from Douglas[7]. Controller costs were estimated.

$$Cost_{Op} = F_I \cdot C_{I,in} \cdot price_{Ini} + F_{m,in} \cdot C_{m,in} \cdot price_{Mon} + F_{cw} \cdot price_{cw} \tag{18}$$

Operating costs, equation (18), included the price of monomer, initiator, and cooling water, Table 4 - Raw material prices.

Table 4 - Raw material prices

Raw Material	Price (USD)
azo-*bis*-Isobutyronitrile($price_{Ini}$)[8]	\$10,550/kg
Methyl Methacrylate($price_{mon}$)[9]	\$1.59/kg
Cooling water($price_{cw}$)[10]	\$343/m^3

Profit was considered to be when the product quality was 25,000 ±100 kg/kmol. The price of acceptable polymer was estimated to be ten times the price of initiator.

Sensitivity to Uncertainty

Finally, it was needed to test model sensitivity to uncertain variables. Uncertain variables were tested individually and in pair combinations to determine which set of uncertainty caused the greatest initial overshoot from the desired quality set point. These combined uncertain variables are then known as a "worst case scenario." Each pair of uncertain variables were tested with each variable being at the highest uncertainty, lowest uncertainty, and mixed combinations of the two.

Case Study

Process Description

The chemical process considered is a free-radical polymerization continuously stirred reactor tank (CSTR).

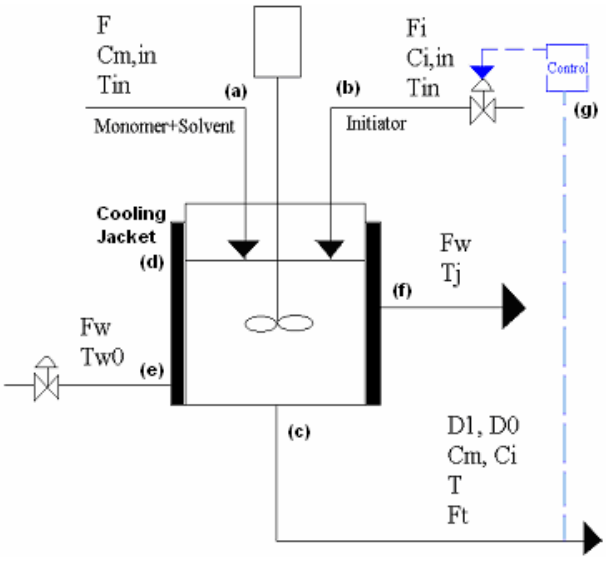

Figure 7 – Case Study: polymerization reactor

Table 5 - Polymerization reactor variables

F	Monomer and solvent flow($m^3 \cdot h^{-1}$)	D_1	Molar density($kmol \cdot m^{-3}$)
F_w	Cooling water flow($m^3 \cdot h^{-1}$)	D_0	Mass density(kgm^{-3})
$C_{m,in}$	Monomer and solvent outlet conc. ($kmol \cdot m^{-3}$)	C_m	Monomer and solvent outlet conc. ($kmol \cdot m^{-3}$)
$C_{I,in}$	Initiator outlet conc. ($kmol \cdot m^{-3}$)	C_I	Initiator outlet conc. ($kmol \cdot m^{-3}$)
F_i	Initiator flow($m^3 \cdot h^{-1}$)	T	Outlet temperature(K)
T_{w0}	Inlet cooling water temperature(K)	T_j	Jacket temperature(K)
T_{in}	Inlet temperature(K)	F_t	Outlet flow($m^3 \cdot h^{-1}$)

The reactor contains two inlets and one outlet. Inlet stream (a) contains the monomer, methyl methacrylate, and the solvent, toluene. Inlet stream (b) contains the initiator, azo-*bis*-isobutyronitrile. The outlet stream (c) contains un-reacted monomer, un-reacted initiator, and the polymer. The reactor is surrounded by a cooling jacket (d) which contains an inlet stream of cooling water (e) and exits the reactor from stream (f). With measurements of the product quality, D_1/D_0, a feedback controller (g) is used to the control the flow of initiator into the reactor so a desired quality could be achieved and maintained. The uncertain variables of the process

were F, T_{w0}, T_{in}, $C_{m,in}$, and $C_{I,in}$. The measured variables were D_1 and D_0. The control variable was F_I.

Mass and Energy Balances

Mass and energy balances can be formulated to describe this system mathematically. The mass equations[2] are as follows in equations (19) through (22).

$$\frac{dC_m}{dt} = -(k_p + k_{f_m}) \cdot C_m \cdot P_0(C_1, T) + \frac{F \cdot (C_{m_{in}} - C_m)}{V} \tag{19}$$

Equation (19) defines the change in the concentration of the monomer over time by finding the difference between the monomer concentration leaving and entering the reactor minus the reaction term. P_0, the rate of reaction as a function of C_I and T, is defined in equation (23) where f* is a dimensionless parameter.

$$\frac{dC_I}{dt} = -k_I \cdot C_I + \frac{F_I \cdot C_{I_{in}} - F \cdot C_I}{V} \tag{20}$$

Equation (20) defines the change in the concentration of the initiator over time by finding the difference between the initiator concentration leaving and entering the reactor minus the reaction term.

$$\frac{dD_0}{dt} = (0.5 \cdot k_{T_c} + k_{T_d}) \cdot [P_0(C_1, T)]^2 + k_{f_m} \cdot C_m \cdot P_0(C_1, T) - \frac{F \cdot D_0}{V} \tag{21}$$

Equation (21) defines the change in molar concentration over time by summing the two reaction terms and subtracting the original molar concentration term.

$$\frac{dD_1}{dt} = M_m \cdot (k_p + k_{f_m}) \cdot C_m \cdot P_0(C_1, T) - \frac{F \cdot D_1}{V} \tag{22}$$

Equation (22) defines the change in mass concentration over time by subtracting the original mass concentration from the reaction term.

$$P_0(C_1,T)=\left(\frac{2\cdot f^*\cdot C_I\cdot k_I}{k_{T_d}+k_{T_c}}\right)^{0.5} \tag{23}$$

Energy equations can also be developed in the same manner as the mass equations and are as follows in equations (24) and (25) where $-\Delta H_P$ is the heat of reaction, ρ is the density of the monomer, C_p is the heat capacity of the monomer, U is the internal energy, A is the area of the reactor, V is the volume of the reactor, F_{cw} is the flow of the cooling water, ρ_w is the density of water, c_w is the heat capacity of water, and V_0 is the volume of the cooling jacket.

$$\frac{dT}{dt}=-k_p\cdot C_m\cdot\frac{(-\Delta H_P)}{\rho\cdot C_p}\cdot P_0(C_1,T)-\frac{U\cdot A}{\rho\cdot C_p\cdot V}(T-T_j)+\frac{F\cdot(T_{in}-T)}{V} \tag{24}$$

Equation (24) defines the change in temperature over time by finding the difference between the temperature leaving and entering the reactor and subtracting the energy leaving through the reactor wall into the cooling jacket as well as the energy created by the reaction.

$$\frac{dT_j}{dt}=\frac{F_{cw}}{V_o}\cdot(T_{w_o}-T_j)+\frac{U\cdot A}{\rho_w\cdot c_w\cdot V_o}(T-T_j) \tag{25}$$

Equation (25) defines the change in jacket temperature over time by finding the difference in temperature of the water entering the reactor and leaving the reactor and adding the energy removed from the reactor through the jacket wall.

The kinetics of the reactions occurring were obtained from previous work[2] and shown in equation (26),

$$k_{i_j} = Z_{i_j} \cdot \exp\left(\frac{-E_{i_j}}{R \cdot T}\right) \tag{26}$$

with R as the Universal Gas Constant, Z_{ij} as the pre-exponential factor, and E_{ij} as the activation energy of the reaction. Kinetic parameters[2] are as follows in Table 6.

Table 6 - Kinetic parameters for k_{Tc}, k_{Td}, k_P, and k_{fm}

i_j	Z_{i_j} Z_{i_j}	E_{i_j}
T_c	3.8223 x 10^{10} kmol·m^{-3}·h	2.9442 x 10^{3} kJ·kmol^{-1}
T_d	3.1457 x 10^{11} kmol·m^{-3}·h	2.9442 x 10^{3} kJ·kmol^{-1}
P	1.7700 x 10^{9} kmol·m^{-3}·h	1.8283 x 10^{4} kJ·kmol^{-1}
f_m	1.0067 x 10^{15} kmol·m^{-3}·h	7.4478 x 10^{4} kJ·kmol^{-1}

Also, the equation for the kinetic coefficient of I, k_I, is shown in equation (27).

$$k_I = A_I \cdot \exp\left(\frac{-E_I}{T}\right) \tag{27}$$

The kinetic parameters for k_I[3] are defined in Table 7 - Kinetic parameters for k_I.

Table 7 - Kinetic parameters for k_I

A_I	E_I
3.7920 x 10^{18} kmol·m^{-3}·h	1.2877 x 10^{5} kJ·kmol^{-1}

Nominal operating conditions and design parameters[2] as seen in Table 8.

Table 8 – Nominal operating conditions and design parameters

F	1.00 m3·h^{-1}
V	0.1 m^3
ρ	866 kg·m^{-3}
$C_{I,in}$	8.0 kmol·m^{-3}
C_p	2.0 kJ·kg^{-1}·K^{-1}
A	2.0 m^2
ρ_w	1000 kg·m^{-3}
V_0	0.002 m^3

F_{cw}	3.26363 m3·h^{-1}
F_I	0.01679 m3·h^{-1}
R	8.314 kJ·kmol^{-1}·K^{-1}
M_m	100.12 kg·kmol^{-1}
$C_{m,in}$	6.0 kmol·m^{-3}
$-\Delta H_P$	57,800 kJ·kmol^{-1}
U	720 kJ·h^{-1}·K^{-1}·m^{-2}
c_w	4.2 kJ·kg^{-1}·K^{-1}
T_{in}	350 K
T_{w0}	293.2 K

Results and Discussion

Steady-State Model

The steady-state models for the isothermal (T=335K) and non-isothermal cases reached equilibrium around the same steady-state values and gave a quality of 24,920 kg·kmol^{-1} and 24,316 kg·kmol^{-1}, respectively.

Table 9 - Steady-state values under steady-state conditions for isothermal and non-isothermal models

Model	C_m (kmol·m^{-3})	C_I (kmol·m^{-3})	D_0 (kmol·m^{-3})	D_1 (kg·m^{-3})	T_j (K)	T (K)
Isothermal	5.5022	0.1329	0.0020	49.8406	-	-
Non-isothermal	5.4900	0.1329	0.0021	51.0645	297.2039	335.3165

The difference in quality between the isothermal and non-isothermal model is due to the steady-state temperature of the non-isothermal model, T=335.3, differs from the steady-state value of the isothermal model, T=335K. Though small, this difference could cause a noticeable change in a system, such as this, that is highly temperature dependent. The temperature of the cooling water, T_j, does not enter into any of the isothermal equations.

Dynamic Model

The steady-state model lacks the ability to show the process under changing conditions that it will inevitably face. A dynamic model was then needed to show this major part of the process. A dynamic model was evaluated for the non-isothermal case with volume of $0.1m^3$ and uncertainty of U_{step}=0.99*U, cmi_{step}=0.985*cmi, and Tin_{step}=0.999*Tin. These uncertainty variables were chosen to represent a model, property, and operation uncertainty, respectively. The isothermal steady-state quality then shifted to 24,513 $kg \cdot kmol^{-1}$ and the non-isothermal steady-state quality to 22,916 $kg \cdot kmol^{-1}$.

Table 10 – Steady-state values under dynamic conditions for isothermal and non-isothermal models

Model	C_m ($kmol \cdot m^{-3}$)	C_I ($kmol \cdot m^{-3}$)	D_0 ($kmol \cdot m^{-3}$)	D_1 ($kg \cdot m^{-3}$)	T_j (K)	T (K)
Isothermal	5.4197	0.1329	0.0020	49.0930	-	-
Non-isothermal	5.3725	0.1327	0.0023	53.8105	297.2513	336.2047

Again, a small change of input temperature greatly shifts the quality of the product in the non-isothermal model as opposed to the small change in the isothermal model due to the highly temperature-dependent nature of the kinetics of the reaction.

P-Controller

The first controller considered was a P-controller.

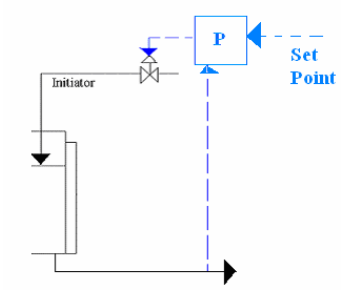

Figure 8 - P-Controller-Single-Input Single Output (SISO) system

The manipulated variable chosen was F_i. The gain was incrementally changed until an approximate optimal response emerged. The non-isothermal dynamic model was used to implement the P-controller (K_c=1x10^{-5}) and then the two models were compared.

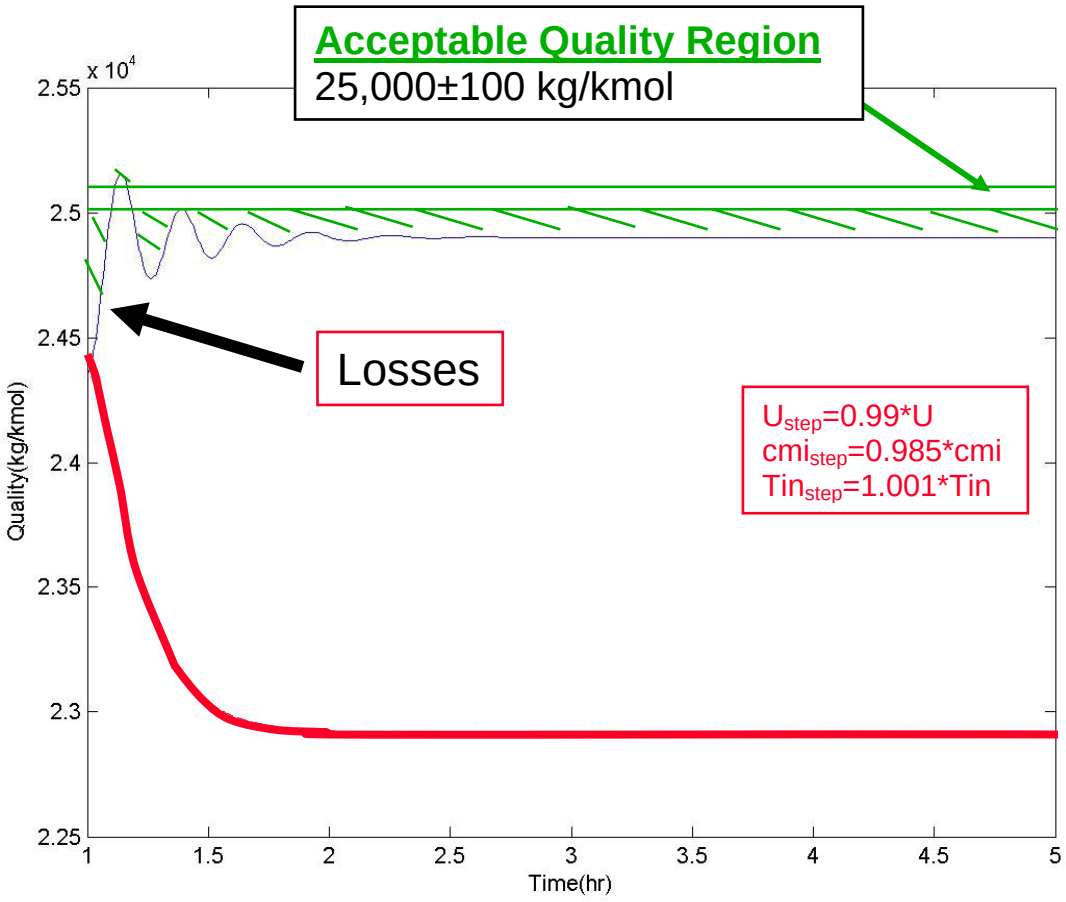

Figure 9 - Non-isothermal dynamic response with P-controller under uncertainty (U_{step}=0.99*U, cmi_{step}=0.985*cmi, and Tin_{step}=0.999*Tin)

While the P-controller greatly corrects the shift in quality, there is still an unacceptable offset from the desired set point of 25,000 ±100 kg/kmol. This controller did not give an acceptable profit due to the product not being within the quality range.

PI-Controller

In order to create no offset a second control scheme, the PI-controller, was added to the non-isothermal dynamic models.

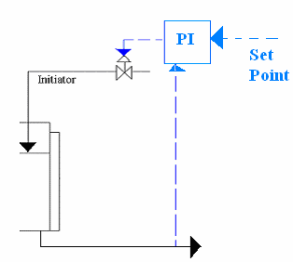

Figure 10 - PI Controller-Single-Input Single-Output (SISO) system

The non-isothermal model can be seen in Figure 11. Each model had the same tuning parameters (Kc = 9.7 x 10^{-6}, τ = 0.99).

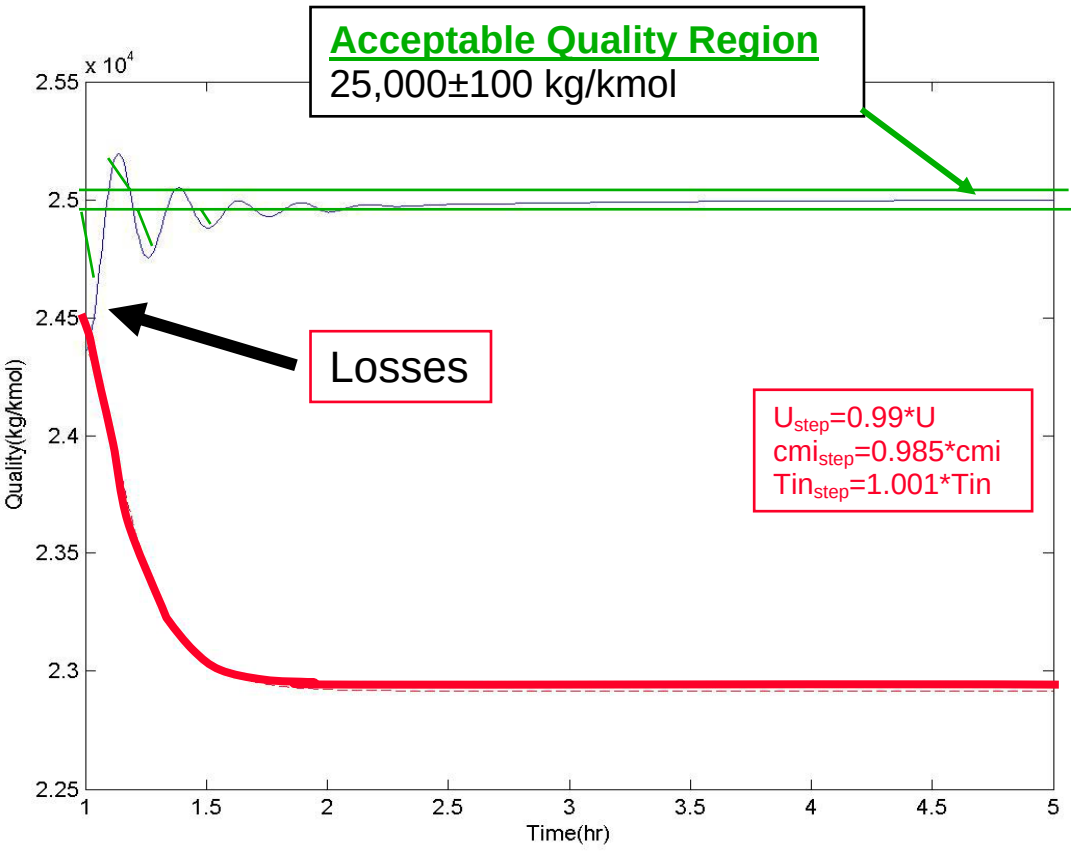

Figure 11 – Non-isothermal dynamic response model with PI-controller under uncertainty (U_{step}=0.99*U,

(cmi_{step}=0.985*cmi, and Tin_{step}=0.999*Tin)

The PI-controller will eventually settle off to the given set-point (no offset) due to its integral action. When compared to the P-controller, the PI-controller reacts less slowly but ultimately will get the product into the desired range.

Tuning Rules

The Ziegler-Nichols and Cohen-Coon Tuning Rules were applied to the open-loop response of the non-isothermal P-controller and PI-controller models. The following data in Table 11 was collected.

Table 11 - Parameters for tuning rules: non-isothermal dynamic open-loop response model with uncertainty (U_{step}=0.99*U, cmi_{step}=0.985*cmi, and Tin_{step}=0.999*Tin)

Model	Δym	SC	K	α	τ
Non-isothermal	$1.475x10^{4}$	0.001	$1.475x10^{6}$	0.06	0.4

By applying the Ziegler-Nichols and Cohen-Coon charts shown earlier in Table 1 and Table 2, respectively, the optimal gain can be calculated.

Table 12 - Comparison of Trial-and-Error Tuning and Tuning Rules: non-isothermal model with uncertainty (U_{step}=0.99*U, cmi_{step}=0.985*cmi, and Tin_{step}=0.999*Tin)

Model	Trial-and-Error Tuning		Ziegler-Nichols Tuning Rules		Cohen-Coon Tuning Rules	
-	K_c	τ_I	K_c	τ_I	K_c	τ_I
P-controller	1×10^{-5}	-	4.52×10^{-6}	-	4.747×10^{-6}	-
PI-controller	9.7×10^{-6}	0.99	4.068×10^{-6}	0.2	1.125×10^{-6}	0.15

Both Ziegler-Nichols and Cohen-Coon tuning parameters differ from the approximate optimal gain found from the P-controller and the PI-controller by about an order of magnitude. This could be explained by the fact that the suggested range for which to use the charts is $0.1<(\alpha/\tau)<1.0$. For this model, the ratio of α/τ comes out to be 0.062. With an approximate

optimal gain established, it was needed to determine the sensitivity of the PI-controller to uncertainty.

IMC Controller

An IMC system was then added to simplify the process of having to optimize two coupled tuning parameters.

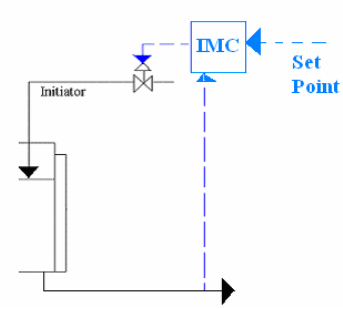

Figure 12 - IMC-Single-Input Single-Output (SISO) system

IMC allowed the process to be tuned around one control parameter, λ, while keeping the same general form of a PI-controller. The response in Figure 13 - Non-isothermal dynamic response model with IMC under uncertainty (U_{step}=0.99*U, cmi_{step}=0.985*cmi, and Tin_{step}=0.999*Tin) was observed.

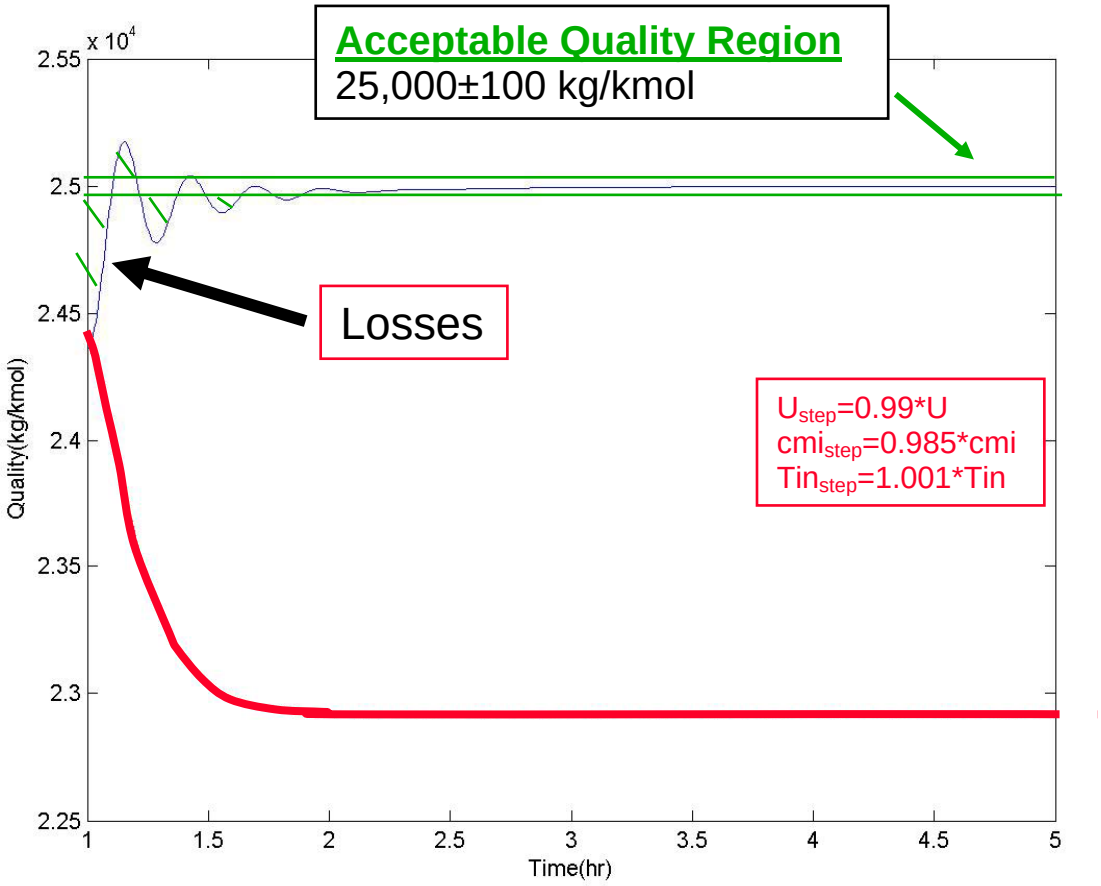

Figure 13 - Non-isothermal dynamic response model with IMC under uncertainty (U_{step}=0.99*U, cmi_{step}=0.985*cmi, and Tin_{step}=0.999*Tin)

While IMC does not greatly out-perform the PI controller, it requires much less work in finding the optimal tuning. A slightly higher profit was seen in the IMC controller than the PI-controller and very significantly higher than the P-controller.

MPC Controller

The last controller considered was MPC.

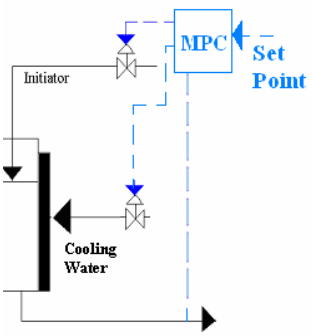

Figure 14- MPC-Single-Input Multiple-Output (SISO) system

MPC was, by far, the most sophisticated control system investigated. Unlike the previous control systems seen MPC has two manipulated variables, F_i and F_{cw}.

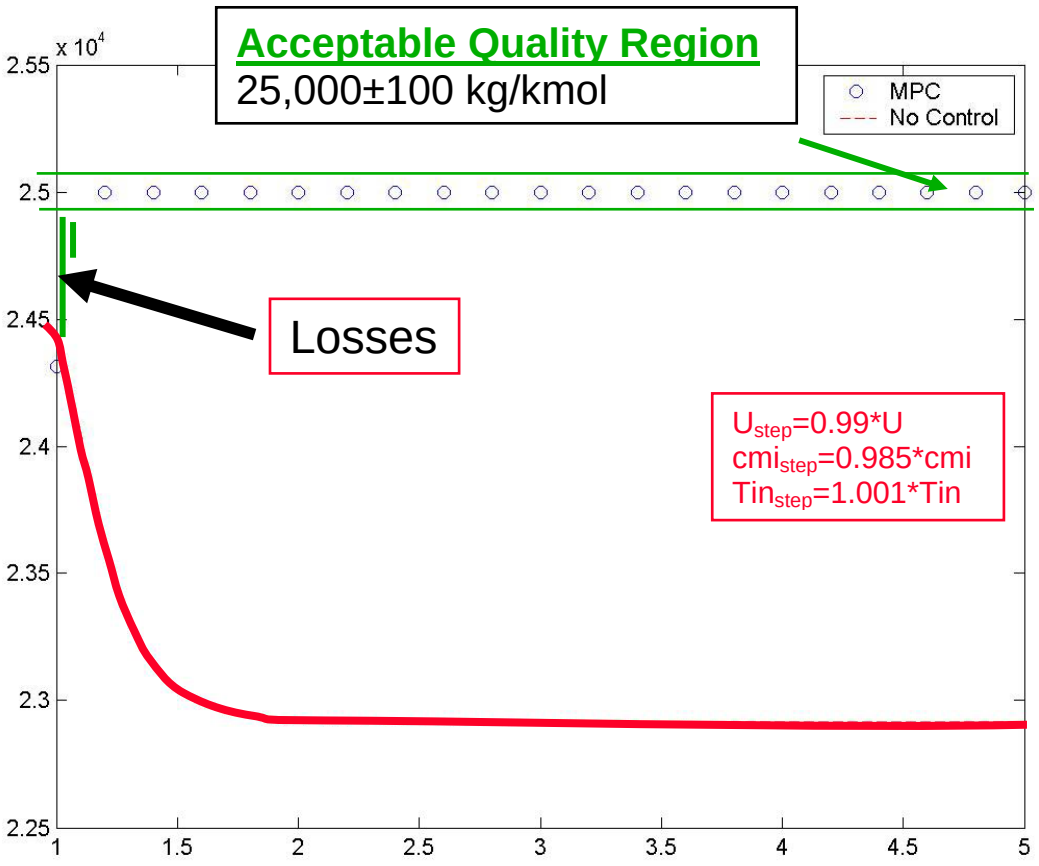

Figure 15- Non-isothermal dynamic response model with MPC under uncertainty (U_{step}=0.99*U, cmi_{step}=0.985*cmi, and Tin_{step}=0.999*Tin)

MPC succeeds where classical control fails by being able to control many different manipulated variables, which often tend to influence each other, and optimize them simultaneously. MPC is also able to significantly raise profits by getting the product in the desired range quickly. MPC outperformed all other classical controllers in these ways.

Cost Model

A quantification of efficiency was needed to compare the controllers. A cost model, including capital, operating, and penalty costs, was used. The penalty costs consisted of the lost input materials when the quality was outside the specified range of 25,000 ±100 kg/kmol. Four different volumes were also tested to determine if a smaller reactor size would be more efficient. All controllers were under an uncertainty (U_{step}=0.99*U, cmi_{step}=0.985*cmi, and Tin_{step}=0.999*Tin).

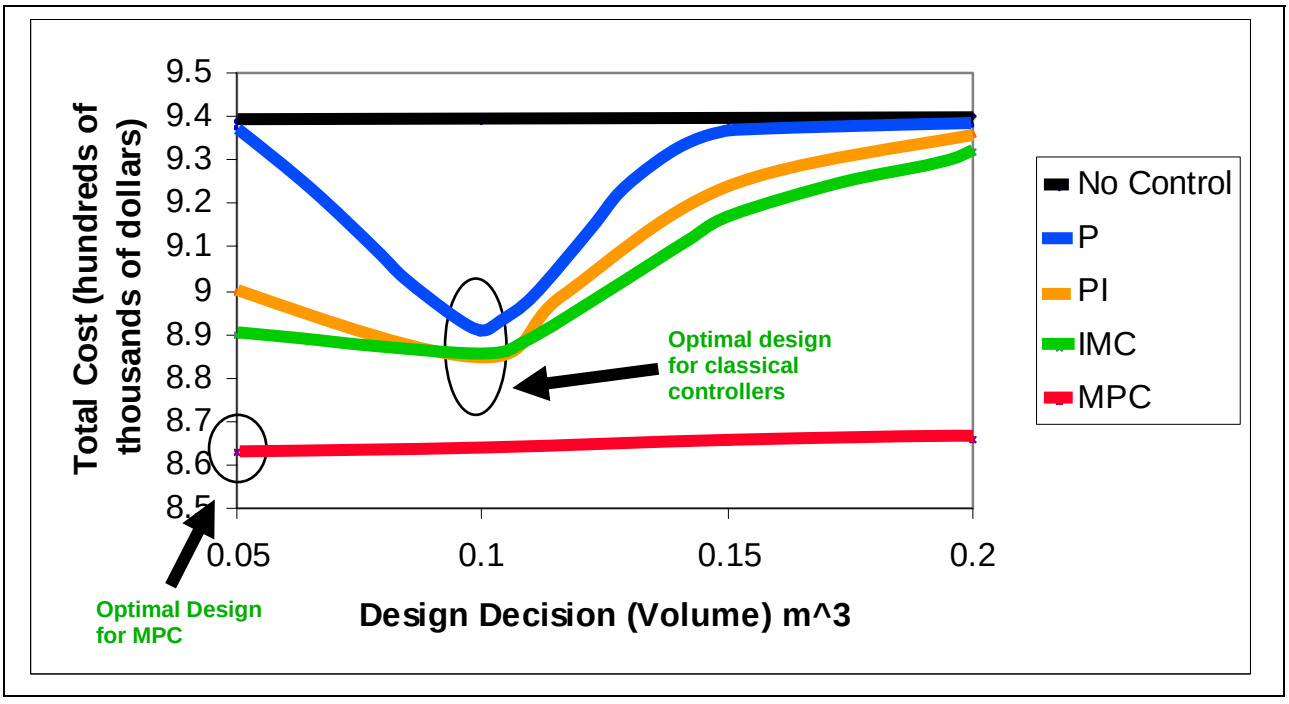

Figure 16 - Cost comparison for control models

The nominal design volume was seen to be $0.1m^3$. From this graph, it can be seen that for a given set of process conditions an optimal reactor size and control scheme not only exist, but more importantly, can be solved for simultaneously using this method.

Table 13 - Cost comparisons for reactor of optimal volume ($V=0.1m^3$) with different controllers

Controller	Capital Cost	Operating Cost	Profit	Total Cost
No Control	$3,362	$934,560	$0	$937,922
P	$3,862	$934,560	$45,169	$892,750
PI	$4,362	$934,560	$52,255	$885,670
IMC	$5,362	$934,560	$52,680	$885,240
MPC	$8,362	$909,600	$52,902	$864,150

It is clear to see that the MPC controller, while having the most capital cost, creates the smallest overall cost for all volumes. A much greater difference between the controllers would be seen if the uncertainty was time-dependant and not represented as a simple step-change but MPC would remain as the optimal choice.

Sensitivity to Uncertainty

The sensitivity of the system was tested by applying disturbances to uncertain variables. It was unfeasible for this project to test all of the combinations of all five uncertain variables so only individual and pair combinations were modeled. Since many of the continuity equations contain temperature terms, it was suspected that the greatest deviation from the desired quality would come from the T_{in}-T_{w0} combination.

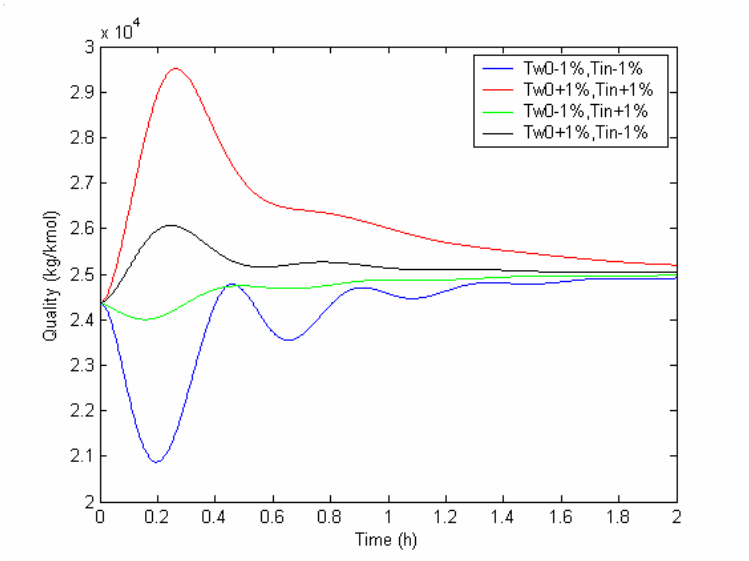

Figure 17 - Sensitivity test of T_{w0} and T_{in} with ±1.0% uncertainty: non-isothermal PI controller

The worst-case scenario of the four possible scenarios would be a positive deviation of both inlet temperature and water temperature followed closely by a negative deviation in both temperature parameters. It was also important to test the sensitivity to a deviation in the concentrations of the monomer and initiator.

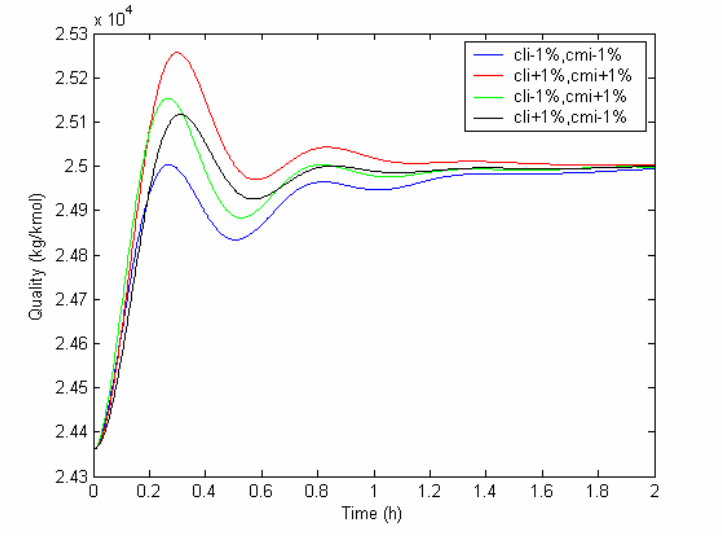

Figure 18 - Sensitivity test of c_{mi} and c_{Ii} with ±1.0% uncertainty: non-isothermal PI controller

A deviation of initiator or monomer concentration does not greatly disturb the system. When compared to the disturbance created by the two temperature variables, this deviation is almost negligible. It is then possible to suggest that this reaction is highly temperature dependant and that the system is most sensitive to the uncertain temperature variables.

Conclusions

While a steady-state model is useful to see small potions of an operating chemical process, a dynamic model is needed to determine the magnitude of the disturbance from uncertainty. While the uncertainty may have a great affect on the performance of a process, a controller with even a small gain can rectify most of the disturbances. More complex control schemes can handle more complex processes with greater disturbances more quickly and accurately, they require greater care with tuning, more computational effort, and greater capital investment. There are many different combinations of tunings so a way to find the optimal tunings is necessary. It is possible to find an approximate optimal gain for a controller by extracting values from the open-loop response of the system and applying the rules set by Ziegler-Nichols and Cohen-Coon. While IMC can be helpful to lessen the difficulty of tuning a PI-controller, MPC still significantly outperforms all classical controllers while also being able to handle many different manipulated variables – a quality which classical controllers lack. To design a more robust system, sensitivity of the process needs to be determined so control can be designed around the "worst-case scenario." The sensitivity is found by measuring the magnitude of the initial overshoot when the uncertain variable is allowed to be at its highest and lowest uncertainty. The data gathered from the sensitivity tests could help influence control decision. For example, since this system seems to be more greatly affected by uncertainty in the

temperature variables, the controller could be set to make greater changes in the control variable when a disturbance in temperature is detected.

Future Work

Future goals for this work would mainly include solving for steady-states of all volumes in the cost model approximation. This would allow for an optimal design to be found at many different process conditions. To better test the robustness of the models, time-dependant uncertainty could be introduced instead of the step changes used in this work. The techniques used by Six Sigma, commonly used to for significant process optimization, would also help to make a more robust process and control system while still reducing total cost by, perhaps, introducing a recycle stream of initiator.

Acknowledgements

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Andrés Malcolm

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Appendix I

Fsolve solves steady-state non-linear problems by taking a guessed initial value, computing the gradient of the result, seeing where it crosses the y-axis, finding a more accurate initial guess, and iterating until the residual comes very close to zero, as can be seen in Figure 19 - Fsolve in Matlab.

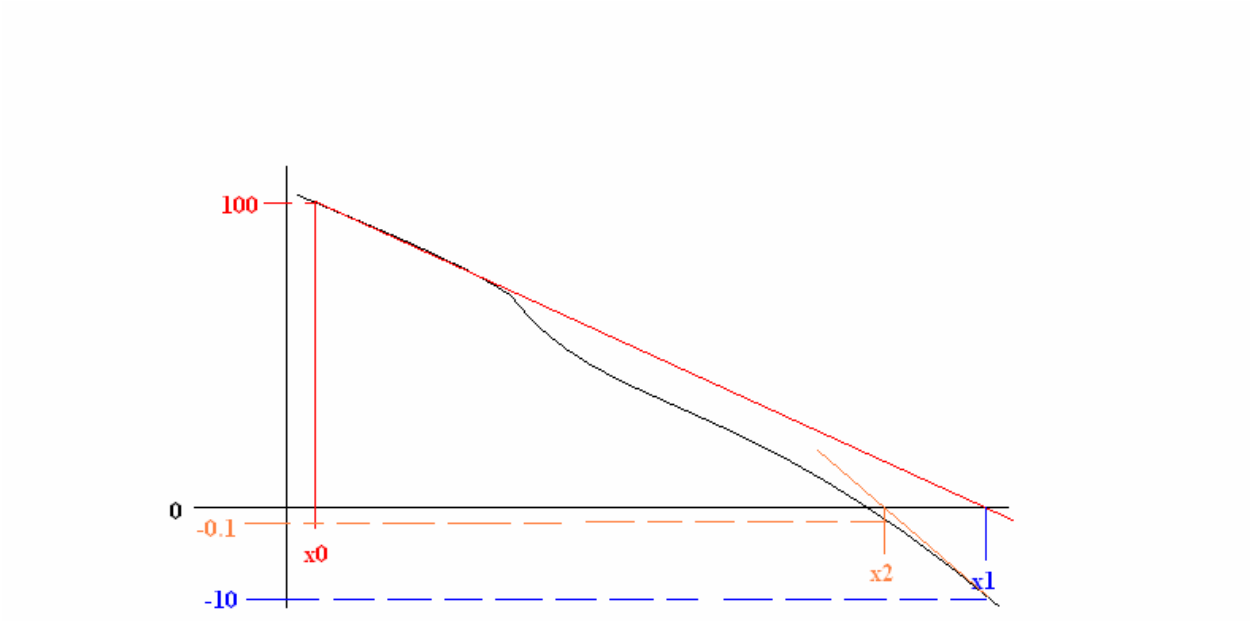

Figure 19 - Fsolve in Matlab

Appendix II – Matlab Code

Steady-state isothermal model

```
function polysolve
clear;
clc;

x0=[5.329,0.1596,0.0024,28.3684]


options=optimset('Display','iter');
[x, residual]=fsolve(@poly1,x0,options);

Cm=x(1);
CI=x(2);
D0=x(3);
D1=x(4);
Tj=305.17;
```

```
T=335;

function res=poly1(x)


Cm=x(1);
CI=x(2);
D0=x(3);
D1=x(4);
Tj=305.17;
T=335;



R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol
F=1.00; %m^3
V=0.1; %m^3
p=866; %kg/m^3
CIin=8; %kmol/m^3
Cp=2; %kJ/(kg*K)
A=2; %m^2
pw=1000; %kg/m^3
Vo=0.02; %m^3
y1sp=25000; %kg/kmol
Fcw=3.26363; %m^3/h
FI=0.01679; %m^3/h
Mm=100.12; %kg/kmol
Cmin=6; %kmol/m^3
Hp=57800; %kJ/kmol
U=720; %kJ/(h*K*m^2)
cw=4.2; %kJ/(kg*K)
Tin=350; %K
y2sp=335; %K
Two=293.2; %K
kTc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
kTd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)
kI=ZI*exp(-EI/(T)); %kmol/(m^3*h)
kP=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)

P0=[2*f*CI*kI/(kTd+kTc)]^0.5;

res(1)=-(kP+kfm)*Cm*P0+F*(Cmin-Cm)/V; %kmol/(m^3*h)
res(2)=-kI*CI+(FI*CIin-F*CI)/V; %kmol/(m^3*h)
res(3)=[0.5*kTc+kTd]*(P0)^2+kfm*Cm*P0-F*D0/V; %kmol/(m^3*h)
res(4)=Mm*[kP+kfm]*Cm*P0-F*D1/V; %kg/(m^3*h)
```

Steady-state non-isothermal model

```
%Steady-state
function polysolve
clear
clc

x0=[5.4900    0.1329    0.0021   51.0645  297.2039  335.3165]


options=optimset('Display','iter');
```

```
[x, residual]=fsolve(@poly1,x0,options);
Cm=(x(1));
CI=(x(2));
D0=(x(3));
D1=(x(4));
Tj=(x(5));
T=(x(6));

Ratio=D1/D0;
Ratio
Cm
CI
D0
D1
Tj
T

function res=poly1(x)

Cm=(x(1));
CI=(x(2));
D0=(x(3));
D1=(x(4));
Tj=(x(5));
T=(x(6));


R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol
F=1.00; %m^3
V=0.1; %m^3
p=866; %kg/m^3
CIin=8; %kmol/m^3
Cp=2; %kJ/(kg*K)
A=2; %m^2
pw=1000; %kg/m^3
Vo=0.02; %m^3
y1sp=25000; %kg/kmol
Fcw=3.26363; %m^3/h
FI=0.01679; %m^3/h
Mm=100.12; %kg/kmol
Cmin=6; %kmol/m^3
Hp=57800; %kJ/kmol
U=720; %kJ/(h*K*m^2)
cw=4.2; %kJ/(kg*K)
Tin=350; %K
y2sp=335; %K
Two=293.2; %K

kTc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
kTd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

kI=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kP=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)



P0=[2*f*CI*kI/(kTd+kTc)]^0.5;
```

```
res(1)=-(kP+kfm)*Cm*P0+F*(Cmin-Cm)/V; %kmol/(m^3*h)
res(2)=-kI*CI+(FI*CIin-F*CI)/V; %kmol/(m^3*h)
res(3)=[0.5*kTc+kTd]*(P0)^2+kfm*Cm*P0-F*D0/V; %kmol/(m^3*h)
res(4)=Mm*[kP+kfm]*Cm*P0-F*D1/V; %kg/(m^3*h)
res(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
res(6)=kP*Cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+F*(Tin-T)/V; %K/h
```

Dynamic isothermal model

```
function[]=PolyReact;

clc;
Fmi=1;
V=0.1;
A=20*V;

ysp=25000;
Tsp=335;

Fi=0.01679;
Fcw=3.26363;

cmi=6;
Tin=350;
U=720;
Hp=57800;
Two=293.2;
Xo=[5.5022    0.1329    0.0020   49.8406]



options0=optimset('Display','iter','MaxFunEvals',1e5);
[Xss]=fsolve(@IsoModelSS,Xo,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,cmi);
Xss;

tend=0.5;
Mstep=tend/1000;
tspan=[0,tend];
options=odeset('Refine',3);
Fmi=Fmi*1.2;

[t,X]=ode15s(@IsoModel,tspan,Xss,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi);

X

cm=X(:,1);
cI=X(:,2);
D0=X(:,3);
D1=X(:,4);
Quality=X(:,4)/X(:,3);

% subplot(3,1,1),plot(t,X(:,1));
% title 'Cm'
% subplot(3,1,2),plot(t,X(:,2));
% title 'CI'
plot(t,Quality)
Legend('PI-controller','No Controller')
hold off;

% Ratio=D1./D0
% plot(t,Ratio,'--r')

function f=IsoModelSS(X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi)

cm=X(1);
cI=X(2);
D0=X(3);
D1=X(4);
```

```
cIi=8;
Mm=100.12;

T=335;
R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)

ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol

ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)
ki=ZI*exp(-EI/T); %kmol/(m^3*h)
kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)

fs=0.58;

cmi=6;
P0=[2*fs*cI*ki/(ktd+ktc)]^0.5;

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(Fi*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f=f';



function dy=IsoModel(t,X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi)

dy=IsoModelSS(X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi);
```

Dynamic non-isothermal model

```
%Dynamic
function[]=PolyNonIso;
clear;
clc;

Fmi=1;
V=0.1;
A=2;

ysp=25000;
Tsp=335;
cIi=8;
cmi=6;
Fi=0.01679;
Fcw=3.26363;

Tin=350;
U=720;
Hp=57800;
Two=293.2;

Xo=[3 0.06 0.0027 16 292 323];

options0=optimset('Display','iter','MaxFunEvals',1e5);
[Xss]=fsolve(@nonIsoModelSS,Xo,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,cmi,cIi);
```

```
Xss;

tend=1;
Mstep=tend/1000;
tspan=[0,tend];
options=odeset('Refine',3);
Fcw=Fcw*1.1;

[t,X]=ode15s(@nonIsoModel,tspan,Xss,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,cmi,cIi);

cm=(X(:,1));
cI=(X(:,2));
D0=(X(:,3));
D1=(X(:,4));
Tj=(X(:,5));
T=(X(:,6));

Ratio=D1./D0;
plot(t,D0,'-b')
X

function f=nonIsoModelSS(X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,cmi,cIi)

cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));

pw=1000;
Vo=0.02;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(Fi*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h
```

```
f=f';



function dy=nonIsoModel(t,X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,cmi,cIi)

dy=nonIsoModelSS(X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,cmi,cIi);
```

P-Controller with cost, V=0.05

```
function[]=PolyReact;

clc;
Fmi=1;
A=2;
V=0.05;
height=V/A;
Aj=0.2*A;
Vo=Aj*height;
ysp=25000;
Tsp=335;

Fi=0.01679;
Fcw=3.26363;

cIi=8;
cmi=6;
Tin=350;
U=720;
Hp=57800;
Two=293.2;
Xo=[5.4900    0.1329    0.0021   51.0645  297.2039  335.3165]

options0=optimset('Display','iter','MaxFunEvals',1e5);
[Xss]=fsolve(@nonIsoModelSS,Xo,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,Tsp,ysp,cmi,cIi,Aj,Vo);
Xss;

tend=5;
Mstep=tend/1000;
tspan=[1:Mstep:tend];
options=odeset('Refine',3);
cmi=cmi*(1-0.015);
U=U*(1-0.01);
Tin=Tin*(1+0.001);


[t,X]=ode15s(@nonIsoModel,tspan,Xss,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)

X;

cm=X(:,1);
cI=X(:,2);
D0=X(:,3);
D1=X(:,4);
Tj=X(:,5);
T=X(:,6);

Kc=0.00001;
SP=25000;
e=D1./D0-SP;
FI=Fi+Kc*e;

Ratio=D1./D0;
plot(t,Ratio,'-b')
hold off;

%Reactor and HE capital
height=V/A;
```

```
Vo=V*0.2;
Aj=Vo/height;

CrBC=9700;
VrBC=0.6057;%m3
CaBC=2500;
Abc=14.40029;

mcIi=cIi*164.21;%mass conc of initiator
mcmi=cmi*100.12;%mass conc of monomer

PriceCW=0.45;%Dol/m3
PricePcont=500;
PricePIcont=1000;
PriceIMC=2000;
PriceMPCpc=5000;
PriceMPCdcs=25000;
PriceSolv=343;
PriceMon=1.59;%Dol/kg
PriceInt=10550;%Dol/kg
SP=25000;
e=Ratio-SP;
costprof=zeros(1,length(t));
   for i=1:length(t);
   if (e(i)<100) & (e(i)>-100)
      costprof(i)=(10*cIi*PriceInt*Fi);
   end
   mFcw(i)=Fcw;
   mFmi(i)=Fmi*mcmi;%mass flow rate
   mFi(i)=Fi*mcIi;%mass flow rate
end



   costcap=CrBC*(V/VrBC)^0.63+CaBC*(Aj/Abc)^0.65
   costprofit=trapz(t,costprof)
   costop=trapz(t,mFi)*PriceInt+trapz(t,mFmi)*PriceMon+trapz(t,mFcw)*PriceCW
   costtotal=costop+costcap-costprofit

function f=nonIsoModelSS(X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)

cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));


pw=1000;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
```

```
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

FI=Fi;

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h

f=f';



function dy=nonIsoModel(t,X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)


cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));
pw=1000;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;
```

```
Kc=0.00001;
SP=25000;
e=D1/D0-SP;
FI=Fi+Kc*e;

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h
dy=f';
```

P-Controller with cost, V=0.1

```
function[]=PolyReact;

clc;
Fmi=1;
A=2;
V=0.1
height=V/A;
Aj=0.2*A;
Vo=Aj*height;
ysp=25000;
Tsp=335;

Fi=0.01679;
Fcw=3.26363;

cIi=8;
cmi=6;
Tin=350;
U=720;
Hp=57800;
Two=293.2;
Xo=[5.4900    0.1329    0.0021   51.0645  297.2039  335.3165]

options0=optimset('Display','iter','MaxFunEvals',1e5);
[Xss]=fsolve(@nonIsoModelSS,Xo,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,Tsp,ysp,cmi,cIi,Aj,Vo);
Xss;

Xdynamic0=[Xss,0];
tend=5;
Mstep=tend/1000;
tspan=[1:Mstep:tend];
options=odeset('Refine',3);
cmi=cmi*(1-0.015);
U=U*(1-0.01);
Tin=Tin*(1+0.001);


[t,X]=ode15s(@nonIsoModel,tspan,Xdynamic0,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)

X;

cm=X(:,1);
cI=X(:,2);
D0=X(:,3);
D1=X(:,4);
Tj=X(:,5);
T=X(:,6);
I=X(:,7);

Kc=0.00000993;
SP=25000;
tau=0.999;
e=D1./D0-SP;
FI=Fi+Kc*(e+(1/tau)*I);
```

```
Ratio=D1./D0;
plot(t,Ratio,'-b')
hold on;

%Reactor and HE capital
height=V/A;
Vo=V*0.2;
Aj=Vo/height;

CrBC=9700;
VrBC=0.6057;%m3
CaBC=2500;
Abc=14.40029;

mcIi=cIi*164.21;%mass conc of initiator
mcmi=cmi*100.12;%mass conc of monomer

PriceCW=0.45;%Dol/m3
PricePcont=500;
PricePIcont=1000;
PriceIMC=2000;
PriceMPCpc=5000;
PriceMPCdcs=25000;
PriceSolv=343;
PriceMon=1.59;%Dol/kg
PriceInt=10550;%Dol/kg
SP=25000;
e=Ratio-SP;
costprof=zeros(1,length(t));
   for i=1:length(t);
   if (e(i)<100) & (e(i)>-100)
      costprof(i)=(10*cIi*PriceInt*Fi);
   end
   mFcw(i)=Fcw;
   mFmi(i)=Fmi*mcmi;%mass flow rate
   mFi(i)=Fi*mcIi;%mass flow rate
end



   costcap=CrBC*(V/VrBC)^0.63+CaBC*(Aj/Abc)^0.65
   costprofit=trapz(t,costprof)
   costop=trapz(t,mFi)*PriceInt+trapz(t,mFmi)*PriceMon+trapz(t,mFcw)*PriceCW
   costtotal=costop+costcap-costprofit

function f=nonIsoModelSS(X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)

cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));


pw=1000;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
```

```
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

FI=Fi;

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h

f=f';



function dy=nonIsoModel(t,X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)


cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));
I=X(7);

pw=1000;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)
```

```
kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

Kc=0.00000993;
SP=25000;
tau=0.999;
e=D1/D0-SP;
FI=Fi+Kc*(e+(1/tau)*I);

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h
f(7)=e;
dy=f';
```

P-Controller with cost, V=0.15

```
function[]=PolyReact;

clc;
Fmi=1;
A=2.8;
V=0.15
height=V/A;
Aj=0.2*A;
Vo=Aj*height;
ysp=25000;
Tsp=335;

Fi=0.01679;
Fcw=3.26363;

cIi=8;
cmi=6;
Tin=350;
U=720;
Hp=57800;
Two=293.2;
Xo=[5.4900    0.1329    0.0021   51.0645  297.2039  335.3165]

options0=optimset('Display','iter','MaxFunEvals',1e5);
[Xss]=fsolve(@nonIsoModelSS,Xo,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,Tsp,ysp,cmi,cIi,Aj,Vo);
Xss;

Xdynamic0=[Xss,0];
tend=5;
Mstep=tend/1000;
tspan=[1:Mstep:tend];
options=odeset('Refine',3);
cmi=cmi*(1-0.015);
U=U*(1-0.01);
Tin=Tin*(1+0.001);


[t,X]=ode15s(@nonIsoModel,tspan,Xdynamic0,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)

X;

cm=X(:,1);
cI=X(:,2);
D0=X(:,3);
D1=X(:,4);
```

```
Tj=X(:,5);
T=X(:,6);
I=X(:,7);

Kc=0.00000643;
SP=25000;
tau=10;
e=D1./D0-SP;
FI=Fi+Kc*(e+(1/tau)*I);

Ratio=D1./D0;
plot(t,Ratio,'-b')
hold on;

%Reactor and HE capital
height=V/A;
Vo=V*0.2;
Aj=Vo/height;

CrBC=9700;
VrBC=0.6057;%m3
CaBC=2500;
Abc=14.40029;

mcIi=cIi*164.21;%mass conc of initiator
mcmi=cmi*100.12;%mass conc of monomer

PriceCW=0.45;%Dol/m3
PricePcont=500;
PricePIcont=1000;
PriceIMC=2000;
PriceMPCpc=5000;
PriceMPCdcs=25000;
PriceSolv=343;
PriceMon=1.59;%Dol/kg
PriceInt=10550;%Dol/kg
SP=25000;
e=Ratio-SP;
costprof=zeros(1,length(t));
   for i=1:length(t);
   if (e(i)<100) & (e(i)>-100)
      costprof(i)=(10*cIi*PriceInt*Fi);
   end
   mFcw(i)=Fcw;
   mFmi(i)=Fmi*mcmi;%mass flow rate
   mFi(i)=Fi*mcIi;%mass flow rate
end



   costcap=CrBC*(V/VrBC)^0.63+CaBC*(Aj/Abc)^0.65
   costprofit=trapz(t,costprof)
   costop=trapz(t,mFi)*PriceInt+trapz(t,mFmi)*PriceMon+trapz(t,mFcw)*PriceCW
   costtotal=costop+costcap-costprofit

function f=nonIsoModelSS(X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)

cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));


pw=1000;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;
```

```
R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

FI=Fi;

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h

f=f';



function dy=nonIsoModel(t,X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)


cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));
I=X(7);

pw=1000;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
```

```
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

Kc=0.00000643;
SP=25000;
tau=10;
e=D1/D0-SP;
FI=Fi+Kc*(e+(1/tau)*I);

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h
f(7)=e;
dy=f';
```

P-Controller with cost, V=0.2

```
function[]=PolyReact;

clc;
Fmi=1;
A=3.5;
V=0.2;
height=V/A;
Aj=0.2*A;
Vo=Aj*height;
ysp=25000;
Tsp=335;

Fi=0.01679;
Fcw=3.26363;

cIi=8;
cmi=6;
Tin=350;
U=720;
Hp=57800;
Two=293.2;
Xo=[5.4900    0.1329    0.0021   51.0645  297.2039  335.3165]

options0=optimset('Display','iter','MaxFunEvals',1e5);
[Xss]=fsolve(@nonIsoModelSS,Xo,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,Tsp,ysp,cmi,cIi,Aj,Vo);
Xss;

tend=5;
Mstep=tend/1000;
tspan=[1:Mstep:tend];
options=odeset('Refine',3);
cmi=cmi*(1-0.015);
U=U*(1-0.01);
Tin=Tin*(1+0.001);
```

```
[t,X]=ode15s(@nonIsoModel,tspan,Xss,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)

X;

cm=X(:,1);
cI=X(:,2);
D0=X(:,3);
D1=X(:,4);
Tj=X(:,5);
T=X(:,6);

Kc=0.00000425;
SP=25000;
e=D1/D0-SP;
FI=Fi+Kc*e;

Ratio=D1./D0;
plot(t,Ratio,'-b')
hold on;

%Reactor and HE capital
height=V/A;
Vo=V*0.2;
Aj=Vo/height;

CrBC=9700;
VrBC=0.6057;%m3
CaBC=2500;
Abc=14.40029;

mcIi=cIi*164.21;%mass conc of initiator
mcmi=cmi*100.12;%mass conc of monomer

PriceCW=0.45;%Dol/m3
PricePcont=500;
PricePIcont=1000;
PriceIMC=2000;
PriceMPCpc=5000;
PriceMPCdcs=25000;
PriceSolv=343;
PriceMon=1.59;%Dol/kg
PriceInt=10550;%Dol/kg
SP=25000;
e=Ratio-SP;
costprof=zeros(1,length(t));
   for i=1:length(t);
   if (e(i)<100) & (e(i)>-100)
      costprof(i)=(10*cIi*PriceInt*Fi);
   end
   mFcw(i)=Fcw;
   mFmi(i)=Fmi*mcmi;%mass flow rate
   mFi(i)=Fi*mcIi;%mass flow rate
end



   costcap=CrBC*(V/VrBC)^0.63+CaBC*(Aj/Abc)^0.65
   costprofit=trapz(t,costprof)
   costop=trapz(t,mFi)*PriceInt+trapz(t,mFmi)*PriceMon+trapz(t,mFcw)*PriceCW
   costtotal=costop+costcap-costprofit

function f=nonIsoModelSS(X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)

cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));
```

```
pw=1000;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

FI=Fi;

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h

f=f';



function dy=nonIsoModel(t,X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)


cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));
pw=1000;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
```

```
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

Kc=0.00000425;
SP=25000;
e=D1/D0-SP;
FI=Fi+Kc*e;

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h
dy=f';
```

PI-Controller with cost, V=0.05

```
function[]=PolyReact;

clc;
Fmi=1;
A=2;
V=0.05;
height=V/A;
Aj=0.2*A;
Vo=Aj*height;
ysp=25000;
Tsp=335;

Fi=0.01679;
Fcw=3.26363;

cIi=8;
cmi=6;
Tin=350;
U=720;
Hp=57800;
Two=293.2;
Xo=[5.4900    0.1329    0.0021   51.0645  297.2039  335.3165]

options0=optimset('Display','iter','MaxFunEvals',1e5);
[Xss]=fsolve(@nonIsoModelSS,Xo,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,Tsp,ysp,cmi,cIi,Aj,Vo);
Xss;

Xdynamic0=[Xss,0];
tend=5;
Mstep=tend/1000;
tspan=[1:Mstep:tend];
options=odeset('Refine',3);
```

```
cmi=cmi*(1-0.015);
U=U*(1-0.01);
Tin=Tin*(1+0.001);


[t,X]=ode15s(@nonIsoModel,tspan,Xdynamic0,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)

X;

cm=X(:,1);
cI=X(:,2);
D0=X(:,3);
D1=X(:,4);
Tj=X(:,5);
T=X(:,6);
I=X(:,7);

Kc=0.000003;
SP=25000;
tau=0.3;
e=D1./D0-SP;
FI=Fi+Kc*(e+(1/tau)*I);

Ratio=D1./D0;
plot(t,Ratio,'-b')
hold off;

%Reactor and HE capital
height=V/A;
Vo=V*0.2;
Aj=Vo/height;

CrBC=9700;
VrBC=0.6057;%m3
CaBC=2500;
Abc=14.40029;

mcIi=cIi*164.21;%mass conc of initiator
mcmi=cmi*100.12;%mass conc of monomer

PriceCW=0.45;%Dol/m3
PricePcont=500;
PricePIcont=1000;
PriceIMC=2000;
PriceMPCpc=5000;
PriceMPCdcs=25000;
PriceSolv=343;
PriceMon=1.59;%Dol/kg
PriceInt=10550;%Dol/kg
SP=25000;
e=Ratio-SP;
costprof=zeros(1,length(t));
   for i=1:length(t);
   if (e(i)<100) & (e(i)>-100)
      costprof(i)=(10*cIi*PriceInt*Fi);
   end
   mFcw(i)=Fcw;
   mFmi(i)=Fmi*mcmi;%mass flow rate
   mFi(i)=Fi*mcIi;%mass flow rate
end



   costcap=CrBC*(V/VrBC)^0.63+CaBC*(Aj/Abc)^0.65
   costprofit=trapz(t,costprof)
   costop=trapz(t,mFi)*PriceInt+trapz(t,mFmi)*PriceMon+trapz(t,mFcw)*PriceCW
   costtotal=costop+costcap-costprofit

function f=nonIsoModelSS(X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)
```

```
cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));


pw=1000;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

FI=Fi;

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h

f=f';



function dy=nonIsoModel(t,X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)


cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));
I=X(7);

pw=1000;
Cp=2;
p=866;
```

```
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

Kc=0.000003;
SP=25000;
tau=0.3;
e=D1/D0-SP;
FI=Fi+Kc*(e+(1/tau)*I);

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h
f(7)=e;
dy=f';
```

PI-Controller with cost, V=0.1

```
function[]=PolyReact;

clc;
Fmi=1;
A=2;
V=0.1
height=V/A;
Aj=0.2*A;
Vo=Aj*height;
ysp=25000;
Tsp=335;

Fi=0.01679;
Fcw=3.26363;

cIi=8;
cmi=6;
Tin=350;
U=720;
Hp=57800;
Two=293.2;
Xo=[5.4900    0.1329    0.0021   51.0645  297.2039  335.3165]
```

```
options0=optimset('Display','iter','MaxFunEvals',1e5);
[Xss]=fsolve(@nonIsoModelSS,Xo,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,Tsp,ysp,cmi,cIi,Aj,Vo);
Xss;

Xdynamic0=[Xss,0];
tend=5;
Mstep=tend/1000;
tspan=[1:Mstep:tend];
options=odeset('Refine',3);
cmi=cmi*(1-0.015);
U=U*(1-0.01);
Tin=Tin*(1+0.001);


[t,X]=ode15s(@nonIsoModel,tspan,Xdynamic0,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)

X;

cm=X(:,1);
cI=X(:,2);
D0=X(:,3);
D1=X(:,4);
Tj=X(:,5);
T=X(:,6);
I=X(:,7);

Kc=0.00000993;
SP=25000;
tau=0.999;
e=D1./D0-SP;
FI=Fi+Kc*(e+(1/tau)*I);

Ratio=D1./D0;
plot(t,Ratio,'-b')
hold on;

%Reactor and HE capital
height=V/A;
Vo=V*0.2;
Aj=Vo/height;

CrBC=9700;
VrBC=0.6057;%m3
CaBC=2500;
Abc=14.40029;

mcIi=cIi*164.21;%mass conc of initiator
mcmi=cmi*100.12;%mass conc of monomer

PriceCW=0.45;%Dol/m3
PricePcont=500;
PricePIcont=1000;
PriceIMC=2000;
PriceMPCpc=5000;
PriceMPCdcs=25000;
PriceSolv=343;
PriceMon=1.59;%Dol/kg
PriceInt=10550;%Dol/kg
SP=25000;
e=Ratio-SP;
costprof=zeros(1,length(t));
   for i=1:length(t);
   if (e(i)<100) & (e(i)>-100)
      costprof(i)=(10*cIi*PriceInt*Fi);
   end
   mFcw(i)=Fcw;
   mFmi(i)=Fmi*mcmi;%mass flow rate
   mFi(i)=Fi*mcIi;%mass flow rate
end
```

```
   costcap=CrBC*(V/VrBC)^0.63+CaBC*(Aj/Abc)^0.65
   costprofit=trapz(t,costprof)
   costop=trapz(t,mFi)*PriceInt+trapz(t,mFmi)*PriceMon+trapz(t,mFcw)*PriceCW
   costtotal=costop+costcap-costprofit

function f=nonIsoModelSS(X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)

cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));


pw=1000;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

FI=Fi;

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h

f=f';



function dy=nonIsoModel(t,X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)


cm=(X(1));
```

```
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));
I=X(7);

pw=1000;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

Kc=0.00000993;
SP=25000;
tau=0.999;
e=D1/D0-SP;
FI=Fi+Kc*(e+(1/tau)*I);

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h
f(7)=e;
dy=f';
```

PI-Controller with cost, V=0.15

```
function[]=PolyReact;

clc;
Fmi=1;
A=2.8;
V=0.15
height=V/A;
Aj=0.2*A;
Vo=Aj*height;
ysp=25000;
Tsp=335;
```

```
Fi=0.01679;
Fcw=3.26363;

cIi=8;
cmi=6;
Tin=350;
U=720;
Hp=57800;
Two=293.2;
Xo=[5.4900    0.1329    0.0021   51.0645  297.2039  335.3165]

options0=optimset('Display','iter','MaxFunEvals',1e5);
[Xss]=fsolve(@nonIsoModelSS,Xo,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,Tsp,ysp,cmi,cIi,Aj,Vo);
Xss;

Xdynamic0=[Xss,0];
tend=5;
Mstep=tend/1000;
tspan=[1:Mstep:tend];
options=odeset('Refine',3);
cmi=cmi*(1-0.015);
U=U*(1-0.01);
Tin=Tin*(1+0.001);


[t,X]=ode15s(@nonIsoModel,tspan,Xdynamic0,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)

X;

cm=X(:,1);
cI=X(:,2);
D0=X(:,3);
D1=X(:,4);
Tj=X(:,5);
T=X(:,6);
I=X(:,7);

Kc=0.00000643;
SP=25000;
tau=10;
e=D1./D0-SP;
FI=Fi+Kc*(e+(1/tau)*I);

Ratio=D1./D0;
plot(t,Ratio,'-b')
hold on;

%Reactor and HE capital
height=V/A;
Vo=V*0.2;
Aj=Vo/height;

CrBC=9700;
VrBC=0.6057;%m3
CaBC=2500;
Abc=14.40029;

mcIi=cIi*164.21;%mass conc of initiator
mcmi=cmi*100.12;%mass conc of monomer

PriceCW=0.45;%Dol/m3
PricePcont=500;
PricePIcont=1000;
PriceIMC=2000;
PriceMPCpc=5000;
PriceMPCdcs=25000;
PriceSolv=343;
PriceMon=1.59;%Dol/kg
PriceInt=10550;%Dol/kg
SP=25000;
```

```
e=Ratio-SP;
costprof=zeros(1,length(t));
   for i=1:length(t);
   if (e(i)<100) & (e(i)>-100)
      costprof(i)=(10*cIi*PriceInt*Fi);
   end
   mFcw(i)=Fcw;
   mFmi(i)=Fmi*mcmi;%mass flow rate
   mFi(i)=Fi*mcIi;%mass flow rate
end



   costcap=CrBC*(V/VrBC)^0.63+CaBC*(Aj/Abc)^0.65
   costprofit=trapz(t,costprof)
   costop=trapz(t,mFi)*PriceInt+trapz(t,mFmi)*PriceMon+trapz(t,mFcw)*PriceCW
   costtotal=costop+costcap-costprofit

function f=nonIsoModelSS(X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)

cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));


pw=1000;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

FI=Fi;

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h
```

```
f=f';



function dy=nonIsoModel(t,X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)


cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));
I=X(7);

pw=1000;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

Kc=0.00000643;
SP=25000;
tau=10;
e=D1/D0-SP;
FI=Fi+Kc*(e+(1/tau)*I);

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h
f(7)=e;
dy=f';
```

PI-Controller with cost, V=0.2

```
function[]=PolyReact;
```

```
clc;
Fmi=1;
A=3.5;
V=0.2
height=V/A;
Aj=0.2*A;
Vo=Aj*height;
ysp=25000;
Tsp=335;

Fi=0.01679;
Fcw=3.26363;

cIi=8;
cmi=6;
Tin=350;
U=720;
Hp=57800;
Two=293.2;
Xo=[5.4900    0.1329    0.0021   51.0645  297.2039  335.3165]

options0=optimset('Display','iter','MaxFunEvals',1e5);
[Xss]=fsolve(@nonIsoModelSS,Xo,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,Tsp,ysp,cmi,cIi,Aj,Vo);
Xss;

Xdynamic0=[Xss,0];
tend=5;
Mstep=tend/1000;
tspan=[1:Mstep:tend];
options=odeset('Refine',3);
cmi=cmi*(1-0.015);
U=U*(1-0.01);
Tin=Tin*(1+0.001);


[t,X]=ode15s(@nonIsoModel,tspan,Xdynamic0,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)

X;

cm=X(:,1);
cI=X(:,2);
D0=X(:,3);
D1=X(:,4);
Tj=X(:,5);
T=X(:,6);
I=X(:,7);

Kc=0.00000993;
SP=25000;
tau=0.999;
e=D1./D0-SP;
FI=Fi+Kc*(e+(1/tau)*I);

Ratio=D1./D0;
plot(t,Ratio,'-b')
hold on;

%Reactor and HE capital
height=V/A;
Vo=V*0.2;
Aj=Vo/height;

CrBC=9700;
VrBC=0.6057;%m3
CaBC=2500;
Abc=14.40029;

mcIi=cIi*164.21;%mass conc of initiator
mcmi=cmi*100.12;%mass conc of monomer
```

```
PriceCW=0.45;%Dol/m3
PricePcont=500;
PricePIcont=1000;
PriceIMC=2000;
PriceMPCpc=5000;
PriceMPCdcs=25000;
PriceSolv=343;
PriceMon=1.59;%Dol/kg
PriceInt=10550;%Dol/kg
SP=25000;
e=Ratio-SP;
costprof=zeros(1,length(t));
   for i=1:length(t);
   if (e(i)<100) & (e(i)>-100)
      costprof(i)=(10*cIi*PriceInt*Fi);
   end
   mFcw(i)=Fcw;
   mFmi(i)=Fmi*mcmi;%mass flow rate
   mFi(i)=Fi*mcIi;%mass flow rate
end



   costcap=CrBC*(V/VrBC)^0.63+CaBC*(Aj/Abc)^0.65
   costprofit=trapz(t,costprof)
   costop=trapz(t,mFi)*PriceInt+trapz(t,mFmi)*PriceMon+trapz(t,mFcw)*PriceCW
   costtotal=costop+costcap-costprofit

function f=nonIsoModelSS(X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)

cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));


pw=1000;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;
```

```
P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

FI=Fi;

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h

f=f';



function dy=nonIsoModel(t,X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)


cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));
I=X(7);

pw=1000;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

Kc=0.00000325;
SP=25000;
tau=2;
e=D1/D0-SP;
FI=Fi+Kc*(e+(1/tau)*I);

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
```

```
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h
f(7)=e;
dy=f';
```

IMC with cost, V=0.05

```
function[]=PolyReact;

clc;
Fmi=1;
A=2;
V=0.05;
height=V/A;
Aj=0.2*A;
Vo=Aj*height;
ysp=25000;
Tsp=335;

Fi=0.01679;
Fcw=3.26363;

cIi=8;
cmi=6;
Tin=350;
U=720;
Hp=57800;
Two=293.2;
Xo=[5.4900    0.1329    0.0021   51.0645  297.2039  335.3165]

options0=optimset('Display','iter','MaxFunEvals',1e5);
[Xss]=fsolve(@nonIsoModelSS,Xo,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,Tsp,ysp,cmi,cIi,Aj,Vo);
Xss;

Xdynamic0=[Xss,0];
tend=5;
Mstep=tend/1000;
tspan=[1:Mstep:tend];
options=odeset('Refine',3);
cmi=cmi*(1-0.015);
U=U*(1-0.01);
Tin=Tin*(1+0.001);


[t,X]=ode15s(@nonIsoModel,tspan,Xdynamic0,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)

X;

cm=X(:,1);
cI=X(:,2);
D0=X(:,3);
D1=X(:,4);
Tj=X(:,5);
T=X(:,6);
I=X(:,7);

L=3;
Kc=1.0746e-5/L;
SP=25000;
tau=0.18;
e=D1./D0-SP;
FI=Fi+Kc*(e+(1/tau)*I);

Ratio=D1./D0;
plot(t,Ratio,'-b')
hold off;

%Reactor and HE capital
height=V/A;
```

```
Vo=V*0.2;
Aj=Vo/height;

CrBC=9700;
VrBC=0.6057;%m3
CaBC=2500;
Abc=14.40029;

mcIi=cIi*164.21;%mass conc of initiator
mcmi=cmi*100.12;%mass conc of monomer

PriceCW=0.45;%Dol/m3
PricePcont=500;
PricePIcont=1000;
PriceIMC=2000;
PriceMPCpc=5000;
PriceMPCdcs=25000;
PriceSolv=343;
PriceMon=1.59;%Dol/kg
PriceInt=10550;%Dol/kg
SP=25000;
e=Ratio-SP;
costprof=zeros(1,length(t));
   for i=1:length(t);
   if (e(i)<100) & (e(i)>-100)
      costprof(i)=(10*cIi*PriceInt*Fi);
   end
   mFcw(i)=Fcw;
   mFmi(i)=Fmi*mcmi;%mass flow rate
   mFi(i)=Fi*mcIi;%mass flow rate
end



   costcap=CrBC*(V/VrBC)^0.63+CaBC*(Aj/Abc)^0.65
   costprofit=trapz(t,costprof)
   costop=trapz(t,mFi)*PriceInt+trapz(t,mFmi)*PriceMon+trapz(t,mFcw)*PriceCW
   costtotal=costop+costcap-costprofit

function f=nonIsoModelSS(X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)

cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));


pw=1000;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
```

```
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

FI=Fi;

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h

f=f';



function dy=nonIsoModel(t,X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)


cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));
I=X(7);

pw=1000;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;
```

```
P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

L=0.08;
Kc=2.5532e-7/L;
SP=25000;
tau=0.18;
e=D1/D0-SP;
FI=Fi+Kc*(e+(1/tau)*I);

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h
f(7)=e;
dy=f';
```

IMC with cost, V=0.1

```
function[]=PolyReact;

clc;
Fmi=1;
A=2;
V=0.1
height=V/A;
Aj=0.2*A;
Vo=Aj*height;
ysp=25000;
Tsp=335;

Fi=0.01679;
Fcw=3.26363;

cIi=8;
cmi=6;
Tin=350;
U=720;
Hp=57800;
Two=293.2;
Xo=[5.4900    0.1329    0.0021   51.0645  297.2039  335.3165]

options0=optimset('Display','iter','MaxFunEvals',1e5);
[Xss]=fsolve(@nonIsoModelSS,Xo,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,Tsp,ysp,cmi,cIi,Aj,Vo);
Xss;

Xdynamic0=[Xss,0];
tend=5;
Mstep=tend/1000;
tspan=[1:Mstep:tend];
options=odeset('Refine',3);
cmi=cmi*(1-0.015);
U=U*(1-0.01);
Tin=Tin*(1+0.001);


[t,X]=ode15s(@nonIsoModel,tspan,Xdynamic0,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)

X;

cm=X(:,1);
cI=X(:,2);
D0=X(:,3);
D1=X(:,4);
Tj=X(:,5);
T=X(:,6);
I=X(:,7);

L=2.1;
```

```
Kc=1.7284e-5/L;
SP=25000;
tau=0.7;
e=D1./D0-SP;
FI=Fi+Kc*(e+(1/tau)*I);

Ratio=D1./D0;
plot(t,Ratio,'-b')
hold on;

%Reactor and HE capital
height=V/A;
Vo=V*0.2;
Aj=Vo/height;

CrBC=9700;
VrBC=0.6057;%m3
CaBC=2500;
Abc=14.40029;

mcIi=cIi*164.21;%mass conc of initiator
mcmi=cmi*100.12;%mass conc of monomer

PriceCW=0.45;%Dol/m3
PricePcont=500;
PricePIcont=1000;
PriceIMC=2000;
PriceMPCpc=5000;
PriceMPCdcs=25000;
PriceSolv=343;
PriceMon=1.59;%Dol/kg
PriceInt=10550;%Dol/kg
SP=25000;
e=Ratio-SP;
costprof=zeros(1,length(t));
   for i=1:length(t);
   if (e(i)<100) & (e(i)>-100)
      costprof(i)=(10*cIi*PriceInt*Fi);
   end
   mFcw(i)=Fcw;
   mFmi(i)=Fmi*mcmi;%mass flow rate
   mFi(i)=Fi*mcIi;%mass flow rate
end



   costcap=CrBC*(V/VrBC)^0.63+CaBC*(Aj/Abc)^0.65
   costprofit=trapz(t,costprof)
   costop=trapz(t,mFi)*PriceInt+trapz(t,mFmi)*PriceMon+trapz(t,mFcw)*PriceCW
   costtotal=costop+costcap-costprofit

function f=nonIsoModelSS(X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)

cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));


pw=1000;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
```

```
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

FI=Fi;

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h

f=f';



function dy=nonIsoModel(t,X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)


cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));
I=X(7);

pw=1000;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol
```

```
ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

L=0.04;
Kc=2.7119e-7/L;
SP=25000;
tau=0.7;
e=D1/D0-SP;
FI=Fi+Kc*(e+(1/tau)*I);

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h
f(7)=e;
dy=f';
```

IMC with cost, V=0.15

```
function[]=PolyReact;

clc;
Fmi=1;
A=2.8;
V=0.15
height=V/A;
Aj=0.2*A;
Vo=Aj*height;
ysp=25000;
Tsp=335;

Fi=0.01679;
Fcw=3.26363;

cIi=8;
cmi=6;
Tin=350;
U=720;
Hp=57800;
Two=293.2;
Xo=[5.4900    0.1329    0.0021   51.0645  297.2039  335.3165]

options0=optimset('Display','iter','MaxFunEvals',1e5);
[Xss]=fsolve(@nonIsoModelSS,Xo,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,Tsp,ysp,cmi,cIi,Aj,Vo);
Xss;

Xdynamic0=[Xss,0];
tend=5;
Mstep=tend/1000;
tspan=[1:Mstep:tend];
options=odeset('Refine',3);
cmi=cmi*(1-0.015);
U=U*(1-0.01);
Tin=Tin*(1+0.001);


[t,X]=ode15s(@nonIsoModel,tspan,Xdynamic0,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)
```

```
X;

cm=X(:,1);
cI=X(:,2);
D0=X(:,3);
D1=X(:,4);
Tj=X(:,5);
T=X(:,6);
I=X(:,7);

L=1;
Kc=0.45/(1.05e6*L);
SP=25000;
tau=0.45;
e=D1./D0-SP;
FI=Fi+Kc*(e+(1/tau)*I);

Ratio=D1./D0;
plot(t,Ratio,'-b')
hold on;

%Reactor and HE capital
height=V/A;
Vo=V*0.2;
Aj=Vo/height;

CrBC=9700;
VrBC=0.6057;%m3
CaBC=2500;
Abc=14.40029;

mcIi=cIi*164.21;%mass conc of initiator
mcmi=cmi*100.12;%mass conc of monomer

PriceCW=0.45;%Dol/m3
PricePcont=500;
PricePIcont=1000;
PriceIMC=2000;
PriceMPCpc=5000;
PriceMPCdcs=25000;
PriceSolv=343;
PriceMon=1.59;%Dol/kg
PriceInt=10550;%Dol/kg
SP=25000;
e=Ratio-SP;
costprof=zeros(1,length(t));
   for i=1:length(t);
   if (e(i)<100) & (e(i)>-100)
      costprof(i)=(10*cIi*PriceInt*Fi);
   end
   mFcw(i)=Fcw;
   mFmi(i)=Fmi*mcmi;%mass flow rate
   mFi(i)=Fi*mcIi;%mass flow rate
end



   costcap=CrBC*(V/VrBC)^0.63+CaBC*(Aj/Abc)^0.65
   costprofit=trapz(t,costprof)
   costop=trapz(t,mFi)*PriceInt+trapz(t,mFmi)*PriceMon+trapz(t,mFcw)*PriceCW
   costtotal=costop+costcap-costprofit

function f=nonIsoModelSS(X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)

cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
```

```
T=(X(6));


pw=1000;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

FI=Fi;

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h

f=f';



function dy=nonIsoModel(t,X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)


cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));
I=X(7);

pw=1000;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
```

```
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

L=0.4;
Kc=0.45/(1.05e6*L);
SP=25000;
tau=0.7;
e=D1/D0-SP;
FI=Fi+Kc*(e+(1/tau)*I);

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h
f(7)=e;
dy=f';
```

IMC with cost, V=0.2

```
function[]=PolyReact;

clc;
Fmi=1;
A=3.5;
V=0.2
height=V/A;
Aj=0.2*A;
Vo=Aj*height;
ysp=25000;
Tsp=335;

Fi=0.01679;
Fcw=3.26363;

cIi=8;
cmi=6;
Tin=350;
U=720;
Hp=57800;
Two=293.2;
Xo=[5.4900    0.1329    0.0021   51.0645  297.2039  335.3165]

options0=optimset('Display','iter','MaxFunEvals',1e5);
[Xss]=fsolve(@nonIsoModelSS,Xo,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,Tsp,ysp,cmi,cIi,Aj,Vo);
Xss;
```

```
Xdynamic0=[Xss,0];
tend=5;
Mstep=tend/1000;
tspan=[1:Mstep:tend];
options=odeset('Refine',3);
cmi=cmi*(1-0.015);
U=U*(1-0.01);
Tin=Tin*(1+0.001);


[t,X]=ode15s(@nonIsoModel,tspan,Xdynamic0,options0,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)

X;

cm=X(:,1);
cI=X(:,2);
D0=X(:,3);
D1=X(:,4);
Tj=X(:,5);
T=X(:,6);
I=X(:,7);

L=2.1;
Kc=1.7284e-5/L;
SP=25000;
tau=0.7;
e=D1./D0-SP;
FI=Fi+Kc*(e+(1/tau)*I);

Ratio=D1./D0;
plot(t,Ratio,'-b')
hold on;

%Reactor and HE capital
height=V/A;
Vo=V*0.2;
Aj=Vo/height;

CrBC=9700;
VrBC=0.6057;%m3
CaBC=2500;
Abc=14.40029;

mcIi=cIi*164.21;%mass conc of initiator
mcmi=cmi*100.12;%mass conc of monomer

PriceCW=0.45;%Dol/m3
PricePcont=500;
PricePIcont=1000;
PriceIMC=2000;
PriceMPCpc=5000;
PriceMPCdcs=25000;
PriceSolv=343;
PriceMon=1.59;%Dol/kg
PriceInt=10550;%Dol/kg
SP=25000;
e=Ratio-SP;
costprof=zeros(1,length(t));
   for i=1:length(t);
   if (e(i)<100) & (e(i)>-100)
      costprof(i)=(10*cIi*PriceInt*Fi);
   end
   mFcw(i)=Fcw;
   mFmi(i)=Fmi*mcmi;%mass flow rate
   mFi(i)=Fi*mcIi;%mass flow rate
end
```

```
   costcap=CrBC*(V/VrBC)^0.63+CaBC*(Aj/Abc)^0.65
   costprofit=trapz(t,costprof)
   costop=trapz(t,mFi)*PriceInt+trapz(t,mFmi)*PriceMon+trapz(t,mFcw)*PriceCW
   costtotal=costop+costcap-costprofit

function f=nonIsoModelSS(X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)

cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));


pw=1000;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

FI=Fi;

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h

f=f';



function dy=nonIsoModel(t,X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,ysp,Tsp,cmi,cIi,Aj,Vo)


cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
```

```
Tj=(X(5));
T=(X(6));
I=X(7);

pw=1000;
Cp=2;
p=866;
cw=4.2;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

L=0.5;
Kc=3.75e-7/L;
SP=25000;
tau=0.7;
e=D1/D0-SP;
FI=Fi+Kc*(e+(1/tau)*I);

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(FI*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h
f(7)=e;
dy=f';
```

PolyMPC2controls with cost

```
function PolyMPC

clear;
clc;

FinalTime=20;
D=1*(.5-rand(1,FinalTime+1));
D=ones(1,FinalTime+1)*.01;

tim=1:0.2:FinalTime/5+1;

u0=[0.01663   0.01663   0.01663     3.3897   3.3897  3.3897];

%SP=1.8;
```

```
% ysp=25000;


for i=1:FinalTime+1
SP(i)=25000+0*i;
end

m=3;% Control horizon
p=10;% Prediction Horizon
tstep=p/200;

A=[];
b=[];
Aeq=[];
beq=[];
lb=[];
ub=[];

options = optimset('Display','off','Diagnostics','off','MaxFunEvals',1e5,'LargeScale','off');

h0=[5.4900    0.1329    0.0021   51.0645  297.2039  335.3165];
for k=1:(FinalTime+1)
   k;
   Prob.user.SP=SP(k);
   Prob.user.D=D(k);
   Prob.user.h0=h0;
   Prob.user.k=k;
    % Call driver routine tomRun, 4th argument > 0 implies call to PrintResult
%    Result  = tomRun(Solver,Prob,0);

   [u,f]= fmincon(@MPCObfminconj,u0,A,b,Aeq,beq,lb,ub,@ODEConstraintsfmincon,options,SP(k),D(k),h0,k,m,p,tstep);

   [t,X]=RealPolyReact(u(1:m),u(m+1:2*m),D(k),m,p,tstep,h0);
   [predt,predX]=PolyReact(u(1:m),u(m+1:2*m),D(k),m,p,tstep,h0);
   Dopt=X(:,4)./X(:,3);
   Dpred=predX(:,4)./predX(:,3);
   for i=1:p % obtain p values from the integration
      g=round(length(t)/p);%
      States(i,:)=X(1+(i-1)*g,:);
   end
   yopt(:,k)=Dopt;
   ypred(:,k)=Dpred;
   yopt(1,:)
   ypred(1,:)
   Fiopt(k)=u(1);
   Fwopt(k)=u(m+1);
   if k>2
    for i=1:m
      u0(i)=Fiopt(k-m+i);
      u0(i+m)=Fwopt(k-m+i);
    end
   end
   h0=States(2,:); %initializes the new integrations with the current states
end

fprintf('\n\n**********Results**********\n')


%[u,f]= fmincon(@MPCObj,u0,A,b,Aeq,beq,lb,ub,@ODEConstraints,options,SP,p,Fcw,m)

%%PLOTS%%%
SP(1:FinalTime+1)=SP;
Dmax(1:FinalTime+1)=26000;
Dmin(1:FinalTime+1)=23000;
% subplot(6,1,1);hold on;
plot(tim,yopt(1,:),'o')
% plot(tim,SP);plot(tim,Dmax,'--');plot(tim,Dmin,'-.');hold off;ylabel('Density');title('+0% mismatch in U');
% subplot(6,1,2);plot(tim,6*(1-0.015)*D,'+');ylabel('Disturbance (Cmi)');
% subplot(6,1,3);plot(tim,350*(1+0.001)*D,'+');ylabel('Disturbance (Tin)');
% subplot(6,1,4);plot(tim,720*(1-0.01)*D,'+');ylabel('Disturbance (U)');
```

```
% Umax(1:FinalTime+1)=.02;
% Umin(1:FinalTime+1)=0.01;
% subplot(6,1,5);hold on;stairs(tim,Fiopt);plot(tim,Umax,'--');plot(tim,Umin,'-.');hold off;ylabel('Control Fi')
% Umax(1:FinalTime+1)=10;
% Umin(1:FinalTime+1)=0;
% subplot(6,1,6);hold on;stairs(tim,Fwopt);plot(tim,Umax,'--');plot(tim,Umin,'-.');hold off;ylabel('Control Fcw')



%Reactor and HE capital
A=2;
V=0.05;
height=V/A;
Vo=V*0.2;
Aj=Vo/height;

CrBC=9700;
VrBC=0.6057;%m3
CaBC=2500;
Abc=14.40029;

Fmi=1;
cmi=6*(1-0.015);
cIi=8;

mcIi=cIi*164.21;%mass conc of initiator
mcmi=cmi*100.12;%mass conc of monomer
Ratio=yopt(1,:);
PriceCW=3.96e-6;%Dol/m3
PricePcont=500;
PricePIcont=1000;
PriceIMC=2000;
PriceMPCpc=5000;
PriceMPCdcs=25000;
PriceSolv=343;
PriceMon=1.59;%Dol/kg
PriceInt=10550;%Dol/kg
SP=25000;
e=Ratio'-SP;
costprof=zeros(1,length(tim));
   for i=1:length(tim);
   if (e(i)<100) & (e(i)>-100)
      costprof(i)=(10*cIi*PriceInt*Fiopt(i));
   end
   mFcw(i)=Fwopt(i);
   mFmi(i)=Fmi*mcmi;%mass flow rate

end

mFi=Fiopt*mcIi;%mass flow rate

   costcap=CrBC*(V/VrBC)^0.63+CaBC*(Aj/Abc)^0.65+PriceMPCpc
   costprofit=trapz(tim,costprof)
   costop=trapz(tim,mFi)*PriceInt+trapz(tim,mFmi)*PriceMon+trapz(tim,mFcw)*PriceCW
   costtotal=costop+costcap-costprofit

% figure(2)
% plot(predt,Dpred)
%
% for i=1:length(t)
%     for j=1:m
%         if t(i)<=j
%         control(i)=u(j);
%         end
%     control(i)=u(m);
%     end
% end
```

MPC-PolyReact

```
function [tt,XX]=PolyReact(Fi,Fcw,D,m,p,tstep,X0);

Fmi=1;
V=0.1;
A=2;

cmi=6*(1-0.015);
Tin=350*(1+0.001);
U=720*(1-0.01);
Hp=57800;
Two=293.2+0*D;
% Xo=[5.4900    0.1329    0.0021   51.0645  297.2039  335.3165];

% options0=optimset('Display','off','MaxFunEvals',1e5);
% [Xss]=fsolve(@nonIsoModelSS,Xo,options0,Fmi,V,A,Fcw0,Fi0,Hp,U,Tin,Two,ysp,cmi);
% Xss;

%Xdynamic0=[Xss,0];
% tend=1;
% Mstep=tend/10;
% tspan=[0:Mstep:tend];
options=odeset('Refine',3);
% control movements
h=0;
for i=1:m; %% simulation in the control horizon
   tspan=[(i-1):tstep:i];
   [t,X]=ode15s(@nonIsoModel,tspan,X0,options,Fmi,V,A,Fcw(i),Fi(i),Hp,U,Tin,Two,cmi);
      for j=1:length(t)
      XX(j+h,:)=X(j,:);
      tt(j+h,:)=t(j);
   end

   h=length(XX);
   X0=X(length(t),:);
end;

%% simulation in the rest of horizon from m to p with the last control action m
tspan=[m:tstep:p];
[t,X]=ode15s(@nonIsoModel,tspan,X0,options,Fmi,V,A,Fcw(m),Fi(m),Hp,U,Tin,Two,cmi);

for j=1:length(t)
    XX(j+h,:)=X(j,:);
    tt(j+h,:)=t(j);
end

function dy=nonIsoModel(t,X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,cmi)

cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));
%I=X(7);

Fmi=1;
pw=1000;
Vo=0.02;
Cp=2;
p=866;
cw=4.2;
cIi=8;
cmi=6;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
```

```
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)


fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

% Kc=0.000009;
% SP=25000;
% tau=0.45;
% e=D1/D0-SP;
% FI=Fi+Kc*(e+(1/tau)*I);

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(Fi*cIi-Fmi*cI)/V; %kmol/(m^3*h)
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h
%f(7)=e;
dy=f';
```

MPC-RealPolyReact

```
function [tt,XX]=RealPolyReact(Fi,Fcw,D,m,p,tstep,X0);

Fmi=1;
V=0.1;
A=2;

cmi=6*(1-0.015);
Tin=350*(1+0.001);
U=720*(1-0.01);
Hp=57800;
Two=293.2+0*D;
% Xo=[5.4900    0.1329    0.0021   51.0645  297.2039  335.3165];

% options0=optimset('Display','off','MaxFunEvals',1e5);
% [Xss]=fsolve(@nonIsoModelSS,Xo,options0,Fmi,V,A,Fcw0,Fi0,Hp,U,Tin,Two,ysp,cmi);
% Xss;

%Xdynamic0=[Xss,0];
% tend=1;
% Mstep=tend/10;
% tspan=[0:Mstep:tend];
options=odeset('Refine',3);
% control movements
h=0;
for i=1:m; %% simulation in the control horizon
   tspan=[(i-1):tstep:i];
   [t,X]=ode15s(@nonIsoModel,tspan,X0,options,Fmi,V,A,Fcw(i),Fi(i),Hp,U,Tin,Two,cmi);
      for j=1:length(t)
      XX(j+h,:)=X(j,:);
      tt(j+h,:)=t(j);
```

```
   end

   h=length(XX);
   X0=X(length(t),:);
end;

%% simulation in the rest of horizon from m to p with the last control action m
tspan=[m:tstep:p];
[t,X]=ode15s(@nonIsoModel,tspan,X0,options,Fmi,V,A,Fcw(m),Fi(m),Hp,U,Tin,Two,cmi);

for j=1:length(t)
    XX(j+h,:)=X(j,:);
    tt(j+h,:)=t(j);
end

function dy=nonIsoModel(t,X,Fmi,V,A,Fcw,Fi,Hp,U,Tin,Two,cmi)

cm=(X(1));
cI=(X(2));
D0=(X(3));
D1=(X(4));
Tj=(X(5));
T=(X(6));
%I=X(7);

Fmi=1;
pw=1000;
Vo=0.02;
Cp=2;
p=866;
cw=4.2;
cIi=8;
cmi=6;
Mm=100.12;

R=8.314; %kJ/(kmol*h)
ZTc=3.8223e10; %kmol/(m^3*h)
ZTd=3.1457e11; %kmol/(m^3*h)
ZI=2.142e18; %1/h
ZP=1.77e9; %kmol/(m^3*h)
Zfm=1.0067e15; %kmol/(m^3*h)
f=0.58;
ETc=2.9442e3; %kJ/kmol
ETd=2.9442e3; %kJ/kmol
EI=1.4897e4; %kJ/kmol
EP=1.8283e4; %kJ/kmol
Efm=7.4478e4; %kJ/kmol


ktc=ZTc*exp(-ETc/(R*T)); %kmol/(m^3*h)
ktd=ZTd*exp(-ETd/(R*T)); %kmol/(m^3*h)

%Calculated using Maner,1996
ki=ZI*exp(-EI/(T)); %kmol/(m^3*h)

kp=ZP*exp(-EP/(R*T)); %kmol/(m^3*h)
kfm=Zfm*exp(-Efm/(R*T)); %kmol/(m^3*h)

fs=0.58;

P0=(2*fs*cI*ki/(ktd+ktc))^0.5;

% Kc=0.000009;
% SP=25000;
% tau=0.45;
% e=D1/D0-SP;
% FI=Fi+Kc*(e+(1/tau)*I);

f(1)=-(kp+kfm)*cm*P0+Fmi*(cmi-cm)/V; %kmol/(m^3*h)
f(2)=-ki*cI+(Fi*cIi-Fmi*cI)/V; %kmol/(m^3*h)
```

```
f(3)=[0.5*ktc+ktd]*(P0)^2+kfm*cm*P0-Fmi*D0/V; %kmol/(m^3*h)
f(4)=Mm*[kp+kfm]*cm*P0-Fmi*D1/V; %kg/(m^3*h)
f(5)=(Fcw/Vo)*(Two-Tj)+(U*A/(pw*cw*Vo))*(T-Tj); %K/h
f(6)=kp*cm*Hp/(p*Cp)*P0-(U*A/(p*Cp*V))*(T-Tj)+Fmi*(Tin-T)/V; %K/h
%f(7)=e;
dy=f';
```