Title
Two Case Studies on the Operational Safety of Chemical Processes via Safeness-Index Based MPC

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Two Case Studies on the Operational Safety of Chemical Processes via Safeness-Index Based MPC

A thesis submitted in partial satisfaction

of the requirements for the degree Master of Science

in Chemical Engineering

by

Carlos Alberto Garcia

2021

ABSTRACT OF THE THESIS

Two Case Studies on the Operational Safety of Chemical Processes

via Safeness-Index Based MPC

by

Carlos Alberto Garcia

Master of Science in Chemical Engineering

University of California, Los Angeles, 2021

Professor Panagiotis D. Christofides, Chair

This work applies a Safeness Index-based model predictive control to explore its benefits in two safety critical chemical processes. The first case study simulates a high-pressure flash drum in tandem with a pressure relief valve. In this simulation the Safeness Index-based MPC is used to maintain the system under safe conditions, avoiding the activation of the pressure relief valve. The second case study simulates 4 units in the Ammonia synthesis process. This work explores the ability of the MPC to mitigate large increases in temperature in the Methanation unit due to decreases in catalytic activity in the high temperature shift reactor. For both cases, a linear dynamic model is identified, and Safeness Index functions and threshold are established.

The thesis of Carlos Alberto Garcia is approved

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Chapter 1

Introduction

Throughout the industry, the continued occurrence of accidents instills the motivation to research methods in which we can improve process operational safety [6]. Various studies have proposed a systems approach on process operational safety [1,12,21]. This has inspired engineers to view incidents as events that take place due to a deviation of the process state to unsafe conditions. A systems perspective can be explored by using the optimization-based feedback control design known as model predictive control (MPC). A MPC makes use of a dynamic process model to make state predictions that are used in optimizing control actions with respect to an objective function [7,8,14,17]. A MPC can be tailored with state constraints to limit deviation into unsafe conditions in the state-space. Coordinating control systems to account for activation of safety systems and safety systems to account for control actuator limitations would shift the industry in safety design for the better. California itself has been home to several accidents. This includes an accident in 2015 at the Exxon refinery in Torrance. The total cost of the accident was estimated in more than $2.4 billion [10]. In this specific accident, there was a malfunction of the emergency system which allowed flammable vapor to leak in the fluidized catalytic cracking unit sending thousands to the hospital. This has been views as the type of accident that could be prevented with coordination between the process control and the emergency safety systems. The control system could safely operate the plant in a limited capacity, while waiting for emergency systems to come back on-line. [13]

In various studies [5,11,15] process control systems have been developed to handle safety in the sense of faults, but without incorporating the safety systems in the design of the control system. Recently [2,19,20] a Safeness Index function can be developed to provide thresholds, that once crossed, trigger safety systems into kicking in. It can also be used as a constraint in the design of the Model Predictive Controller (MPC) providing some coordination between the control and the safety systems.

In this work we explore two safety critical chemical processes. The goal of this work is to develop and apply a Safeness Index-based Model Predictive Controller (MPC) to both chemical processes and demonstrate what benefit there is. For both case studies, the first step is identifying a linear dynamic model from nominal process data. A Safeness Index function and Safeness Index threshold is then developed taking account of both the state variable and the safety system characteristics. The safeness index is then integrated into the MPC as a soft constraint implementing slack variables when the state is outside the region of safe operation. After developing the MPC with Safeness Index considerations, the system is validated using a co-simulation of MATLAB and Aspen. Through these simulations we can test if the MPC can either avoid activating safety systems when disturbances are introduced or at least work together with the safety systems to lessen the unsafe state.

Chapter 2

Flash Drum process and Control Objectives

2.1 Process Description

A flash drum is commonly used in industry to separate mixtures of varying components into a liquid and a vapor stream. The components are separated due to the differences in vapor pressures between each component. As seen in the figure, a liquid feed with flow rate F, mole fraction z_i of component i, temperature T_f and pressure P_f passes through a heat exchanger using a heating duty of Q exiting with a new temperature and pressure T_{in} and P_{in} respectively. As the feed passes through a throttling valve, the feed is separated adiabatically into a liquid stream L and a vapor stream V with compositions x_i and y_i respectively. For this case study the feed temperature is 40ºC, the feed pressure is 45 bar, the flash drum height is 4 ft, and drum diameter is 1 ft. The feed composition entering the flash drum is of the composition 10% methane, 20% ethane, 30% propane, 35% butane, and 5% pentane.

Aspen Plus Dynamics software was used to dynamically simulate and model the flash process under the parameters that have been described. This allowed for dynamic calculations of component molar balances, energy balances, dynamic changes in the state variables of the drum pressure and temperature, and the molar composition of the vapor and liquid phases.

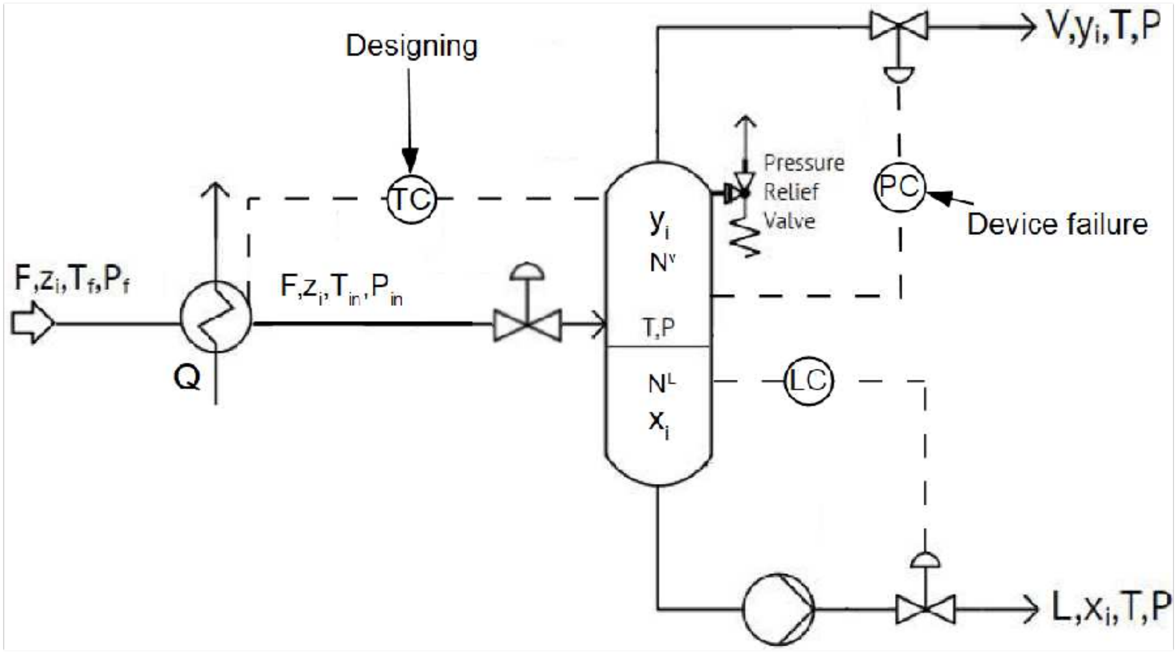

Figure 1: A schematic of the flash process

During safe conditions, controllers are used to maintain the drum pressure around a desired value. Under proper operation of the equipment, two controllers are used to control the liquid effluent valve and vapor effluent valve to sustain the desired the drum liquid level and drum pressure respectively. In cases where the system is not functioning properly, a pressure relief valve is integrated to avoid dangerous outcomes that may arise. Such malfunctioning equipment can include the accidently closure of either effluent valve or a broken pressure sensor that could lead to improper control actions.

Pressure relief valves are a type of safety valve used to control or limit the pressure in a system in case of an overpressure event. The pressure relief valve was also simulated using Aspen Plus, allowing for proper sizing and calculation of the dynamics. For this case study, the pressure relief valve is designed for a situation in which the top vapor valve is totally closed due to control failure. Aspen Plus calculated that the minimum relief flow required to guarantee device safety to be 523 kg/h. To meet this relief flow, a standardized orifice size of 8.303 cm^2 was used in our case study.

Since the operating pressure is 10 bar and the maximum durable pressure of the flash drum is 12 bar, 10.5 bar has been chosen as the opening pressure of the pressure relief valve. The resetting pressure is set to 9 bar so that the relief valve does not close until the event has settled. Exiting the relief valve is assumed to be only vapor and flash calculations of the drum are made under constant enthalpy.

2.2 Control Objective

For this case study the flash drum begins at the operating steady state under the influence of a Model Predictive Controller (MPC). The malfunction to be introduced is the accidental closure of the vapor effluent valve. This is simulated by closing the vapor effluent valve from 50% to a smaller opening. The expected result is an immediate increase in pressure and temperature in the flash drum.

The objective of the control system is to keep the temperature within the drum at a desired set-point and to prevent the relief valve opening due to a small disturbance. The heating duty Q is the manipulated variable of the control system. The controller was designed to be able to deal with the vapor effluent valve being closed from 50% to 35%. Thus, within this range the temperature will be controlled by the manipulation of the heating duty. Going below 35% should trigger the relief valve and work safely with the controller to remain below the maximum operating pressure of 12 bar.

Chapter 3

Safeness Index-based Model Predictive Control: Case Study 1

3.1 Model Identification

The first case study simulates with Aspen Plus Dynamics a flash drum with steady state temperature $T_s = 25°\text{C}$ and $P_s = 10$ bar. The steady state heating duty, our input, is Q_s = 87.6 kW. So that the equilibrium point of the system lies at the origin of the state-space, we use deviations variable in the form of $x^T = [T - T_s \; P - P_s]$ and $u = Q - Q_s$. To incorporate a model predictive control, a process model of the flash drum is required to predict future states. To identify such model, data on temperature and pressure was generated from the Aspen open-loop simulation with pseudorandom binary sequence (PRBS) signal in heating duty Q. Then using a Multivariable Output Error State Space (MOSEP) algorithm in MATLAB we can identify a model of the form

$$\frac{dx}{dt} = Ax + Bu \quad (1)$$

$$A = \begin{bmatrix} -0.047453 & -0.22548 \\ -0.001111 & -0.097369 \end{bmatrix} \qquad B = \begin{bmatrix} 0.01488 \\ 0.002277 \end{bmatrix}$$

3.2 Designing of the Safeness Index

Safeness Index is a function of the process state and is an indication of the safeness of the plant. It considers the interaction between several variables, as well as the interaction between units in a plant [2] Due to its ability to account for interactions between states, a state-based index indicates a process becoming unsafe in a gradual way [12] instead of crossing safety threshold abruptly.

As high temperature and pressure are strong safety factors, the Safeness Index must be designed so that these factors are characterized as unsafe conditions. And that any temperature and pressure combination that falls below the steady state values are characterized as safe. To capture both these characteristics we must set the Safeness Index to be zero if both state variables are negative and positive if either state variable is positive. The Safeness Index can then be represented by the following form:

$$f^{+}(x) = \begin{cases} 0, & x < 0 \\ x, & x \geq 0 \end{cases} \quad (2)$$

$$S(x) = k_T \left[f^{+}\left(\frac{x_1}{T_S}\right)\right]^2 + k_P \left[f^{+}\left(\frac{x_2}{P_S}\right)\right]^2 \quad (3)$$

Where k_T and k_P are the weights for the temperature and pressure respectively. The state variables are divided by their steady state values in order normalize the variables to eliminate the effect any difference in magnitude that may arise. The quadratic form of S(x) ensures that any deviation from the steady state will have a significant effect on the value of the Safeness Index. In our flash drum system, an increase in pressure is more hazardous than an increase in temperature. Therefore, for our safeness index we will put more weight on the pressure term of the index; $k_T = 1000$ and $k_P = 3000$. Additional, though the Safeness Index has a quadratic form it serves a different function compared to a Lyapunov function. Where a Lyapunov function is used to ensure closed loop stability, the Safeness Index is used to indicate process safety.

In designing the Safeness Index, it was important to choose a threshold value S_{TH} that would avoid triggering the safety relief valve. Considering the possibility of model mismatch and the sample-and-hold implementation of the controller, the threshold must be more conservative to allow for overshoot of the Safeness Index. To set a threshold, we first calculated S(x) when the relief valve is activated at 10.5 bar; $S([0\ 0.5]^T) = 7.5$. To be conservative the threshold is chosen as $S_{TH} = 6$.

3.3 Safeness Index-based Model Predictive Controller

The Safeness Index-based MOC is given by the following optimization problem:

$$\min_{u \in S(\Delta), y} \int_{t_k}^{t_{k+N}} \left(\|\tilde{x}_1(\tau)\|_{Q_c}^2 + \|u(\tau)\|_{R_C}^2 \right) d\tau + \sum_{i=1}^{N} k_1 e^{-k_2 y(i)}, k_1, k_2 > 0 \tag{4a}$$

$$\text{s.t} \qquad \dot{\tilde{x}}(t) = A\tilde{x}(t) + Bu(t) \tag{4b}$$

$$\tilde{x}(t_k) = x(t_k) \tag{4c}$$

$$u(t) \in U, \forall t \in [t_k, t_{k+N}] \tag{4d}$$

$$S\left(\tilde{x}(t_k + i)\right) + y(i) \leq S_{TH},\ i = 1,2, \dots, N \tag{4e}$$

$$y(i) \in R,\ i = 1,2, \dots, N, \quad if\ S\left(x(t_k)\right) > S_{TH} \tag{4f}$$

$$y(i) \geq 0,\ i = 1,2, \dots, N, \quad if\ S\left(x(t_k)\right) \leq S_{TH} \tag{4g}$$

where $\tilde{x}$ is the predicted state trajectory, $S(\Delta)$ is the set of piecewise constant functions with period Δ, and N is the number of sampling periods in the prediction horizon. The value u*(t), calculated over the entire prediction horizon $t \in [t_k, t_{k+N}]$, is the optimal input trajectory of the Safeness Index-based MPC optimization problem. The control input calculated for the first sampling period in the prediction horizon $u^*(t_k)$ is applied to the first sampling period and the MPC problem is resolved at the next sampling period. Equation (4a) is minimizing the integral of $\|\tilde{x}_1(\tau)\|_{Q_c}^2 + \|u(\tau)\|_{R_C}^2$ over the prediction horizon and the penalty term $\sum_{i=1}^{N} k_1 e^{-k_2 y(i)}$ with the slack variable y(i). As the flash drum temperature T is the only state variable that is being controlled, it is the sole state variable in the integral. Equation (4b) is the linear model of equation (1) that is used to predict the states within the closed-loop system. Equation (4c) is the state initial condition of the optimization problem, evaluated at $t = t_k$. Equation (4d) is simply the input constraint, the range of heating duty that can be applied to the system. Equation (4e) is the Safeness Index constraint, that keeps the index below the threshold S_{TH} with the slack variable y(i). The soft constraint allows for a gradual change in input as the index gets close to the threshold. When the index is below the threshold, nonnegative slack variables ensure that the constraint (4e) holds. And when the index is above the threshold, negative slack variable ensure that the constraint (4e) still holds. The parameters k_1 and k_2 should be chosen carefully such that the slack variables have little effect through the penalty term in equation (4a) when below the threshold and significant effect when above the threshold. For this case study parameters k_1 and k_2 are 90 and 1.6 respectively.

The optimization problem of the Safeness Index-based MPC of equation 4 was solved using the solver FilterSD on OPTI Toolbox in MATLAB; sampling period 0.5s and prediction horizon N = 10. Then explicit Euler was used to integrate the dynamic model; step size 10^{-3}.

Chapter 4

Simulation Results: Case Study 1

4.1 Simulation without relief valve activation

The first disturbance that was applied to the flash drum system closed the top vapor effluent valve from 50% to 45%. Due to this disturbance, both pressure and temperature increase as was expected. In response to this increase in temperature and pressure, the Safeness Index-based MPC tries minimizing the objective function of equation (4a). As the only input variable we have control over is the heat duty, the controller responses with a decrease in Q. This in turn lowers the increasing temperature and stabilizes the pressure from increasing further as can be seen in the following figure.

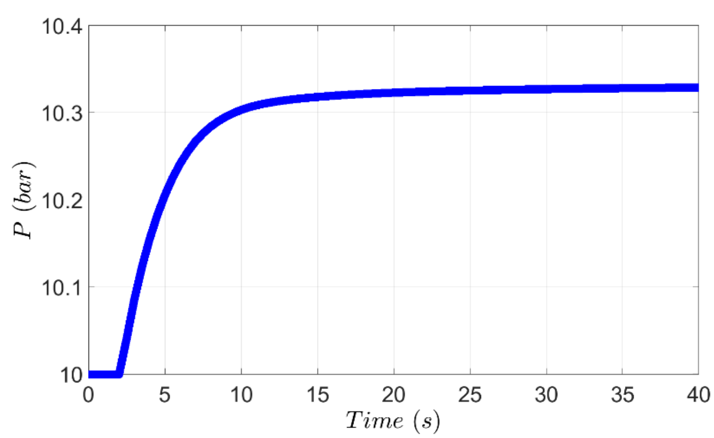

Figure 2: Drum Pressure when the top vapor valve is closed from 50% to 45%

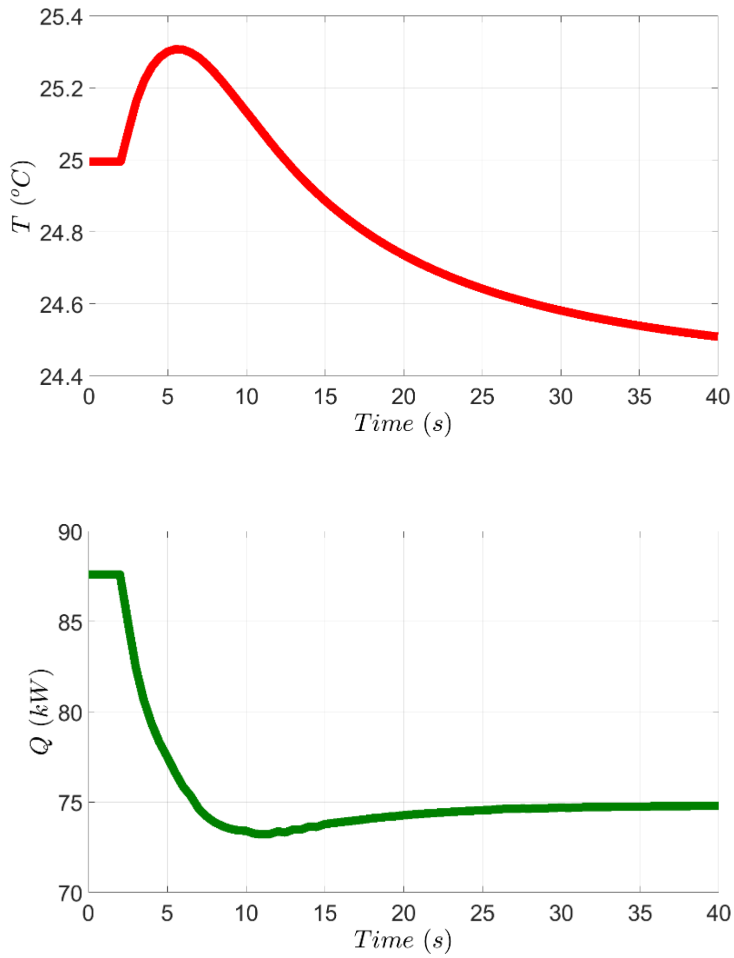

Figure 3: Input and Temperature profiles when the top vapor valve is closed from 50% to 45%

As there was an increase in both temperature and pressure, there would of course be an increase in the Safeness Index. Though an increase in Safeness Index indicates a transition towards unsafe states, the respond of the MPC prevents the index from getting any closer to the threshold. It must be mentioned that the purpose of the MPC is to keep the system away from states that are considered unsafe. Though the system was not able to return to the original state, the MPC was able to stabilize the Safeness Index below the threshold; $S_{TH} = 6$. As can be seen in the figure below.

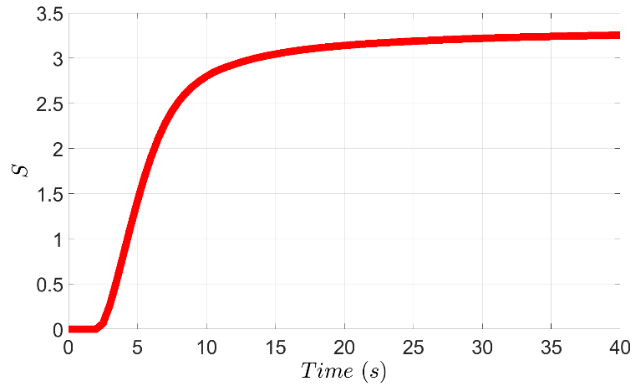

Figure 4: Safeness Index profile when the top vapor valve is closed from 50% to 45%

Next, the vapor effluent valve is closed to 35% open. This disturbance is met with an immediate increase in temperature and pressure, and in turn a large increase in the Safeness Index. As the Safeness Index quickly increases towards the threshold, the MPC aggressively decreases heat duty Q to prevent exceeding 10.5 bar. Though the safeness index does surpass the threshold for a few seconds, the drastic decrease in duty is able to keep the pressure in check and prevent it from exceeding 10.5 bar and activating the relief valve. As the system stabilizes, the Safeness index returns to below the threshold $S_{TH} = 6$. Note that as the safeness index approaches the threshold, the Safeness Index-based MPC drops the heat duty to its lower bound of 0 kW.

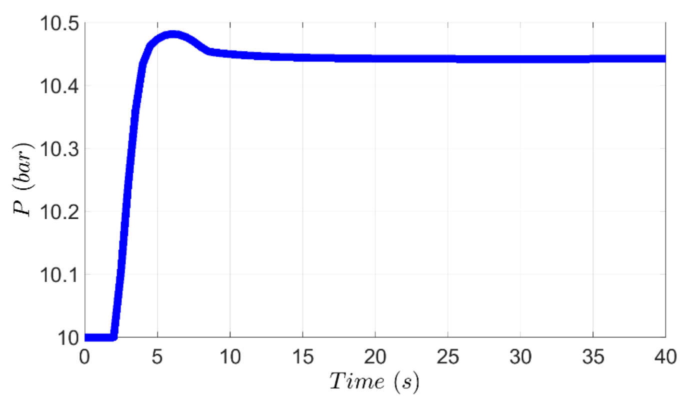

Figure 5: Drum pressure profiles when the top vapor valve is closed from 50% to 35%

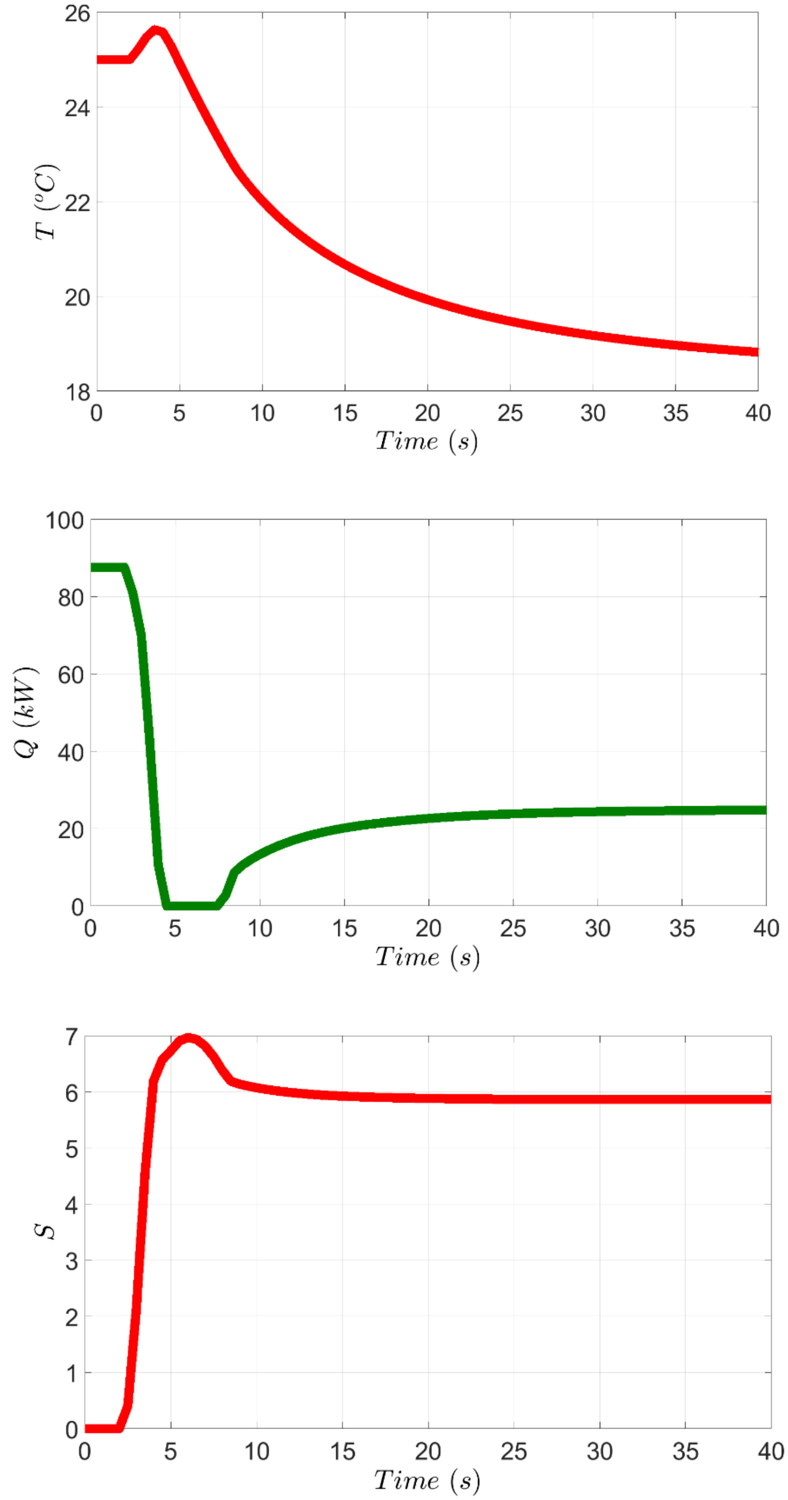

Figure 6: Temperature, Input, and Safeness Index profiles when the top vapor is closed from 50% to 35%

4.2 Simulation with relief valve activation

In introducing a large disturbance, the system is unable to mitigate or prevent high pressure build up in the flash drum. For this disturbance the vapor effluent valve is changed from 50% to 10% open. This is met with an immediate increase in temperature and pressure. The safeness index quickly surpasses the threshold, and the pressure quickly exceeds the relief valve activation pressure of 10.5 bar. The Safeness index MPC quickly sets the heat duty to its lower bound just as it did in the 35% simulation, however it was not able to prevent the relief valve activation. Thus in the figures below you see a quick increase in pressure and then a sudden drop in pressure as the relief valve is activated. After the relief valve is closed, the Safeness Index-based MPC drives the process states back to the steady-states.

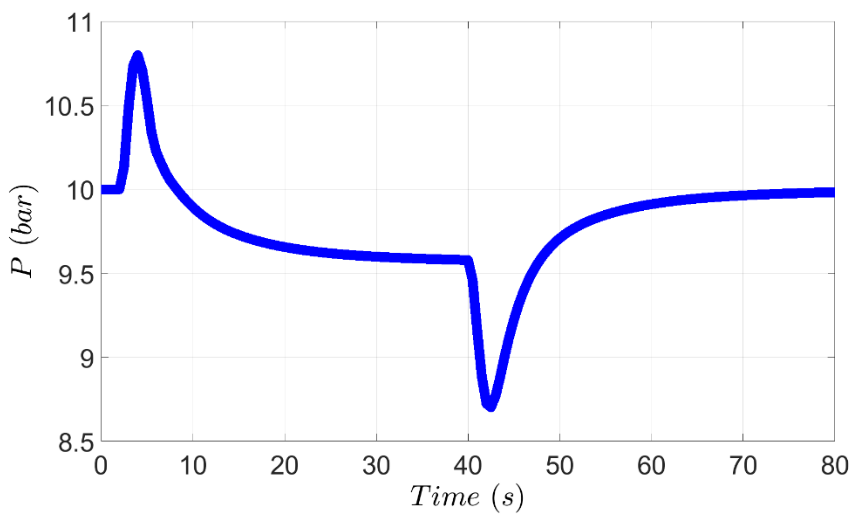

Figure 7: Drum pressure profile when the top vapor valve is closed from 50% to 10%

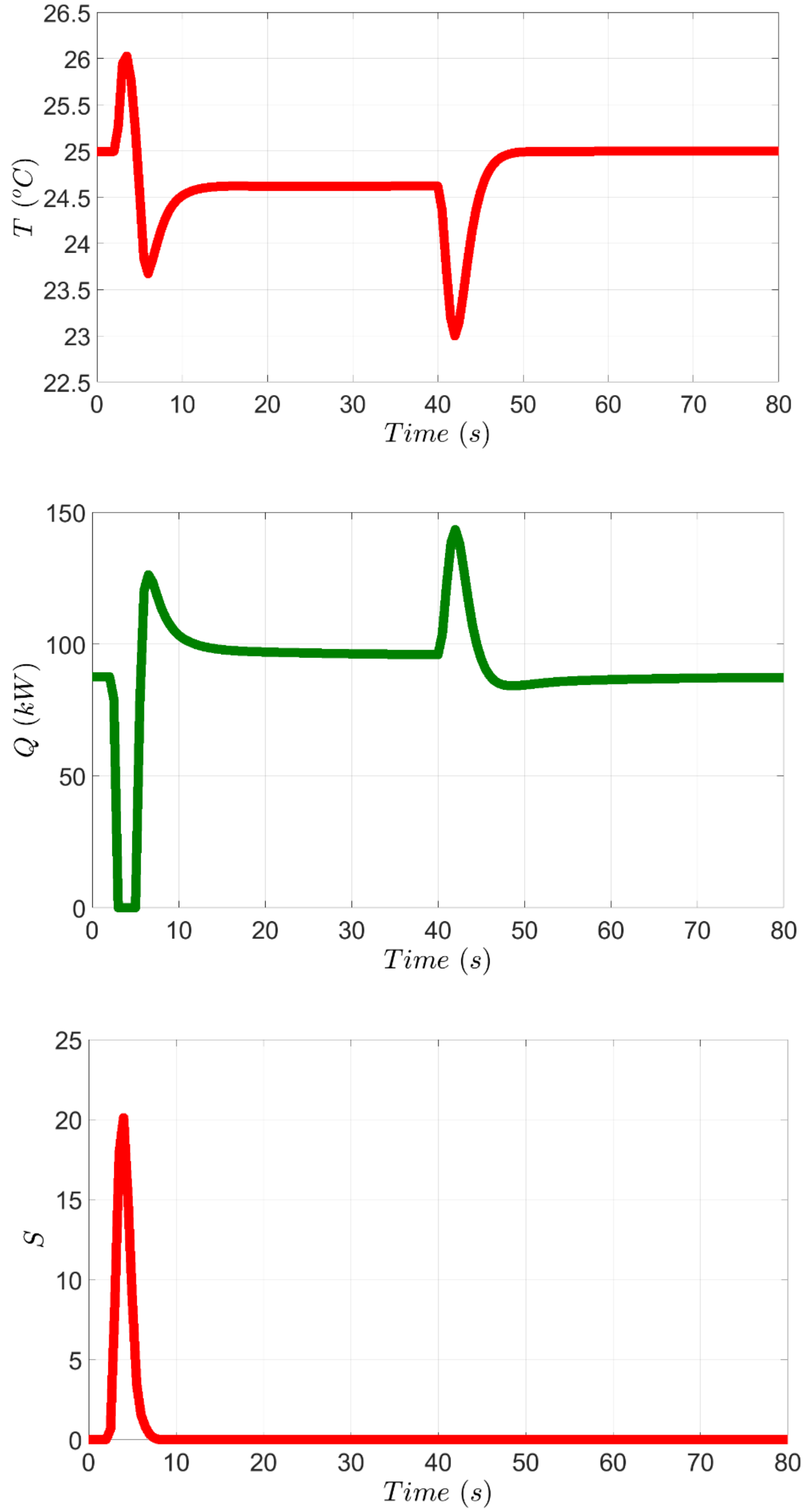

Figure 8: Temperature, input, and safeness index profiles when top vapor valve closed 50% to 10%

Chapter 5

The Ammonia Process

5.1 Process Description

Case study two focuses on three units of the ammonia synthesis process: shift conversion, carbon dioxide removal and methanation. All three units are used to remove carbon monoxide and carbon dioxide, products that are produces by the steam reforming unit. This is to avoid the poisoning of the ammonia synthesis catalyst [3]. The smallest amount of carbon monoxide and carbon dioxide in the synthesis gas is able to denature the catalyst used in ammonia synthesis.

The shift conversion section consists of a high temperature shift reactor and a low temperature shift reactor. These are two adiabatic tube reactors that convert carbon monoxide and water into carbon dioxide and hydrogen. Each shift reactor has a bed of catalyst and operate at different temperatures. The high temperature and low temperature shift reactor typically operates at a temperature of around 400ºC and 200ºC respectively. The high temperature shift reactor reduces the carbon monoxide down to about 2-4%. The low temperature shift reactor can reduce carbon monoxide content between 0.1-0.3% [3,9,18].

Upon leaving the shift conversion section, the case is purified in the adsorption column to remove carbon dioxide and water vapor. Following is the methanation unit that is used to remove trace amounts of carbon monoxide and carbon dioxide. In this unit the concentrations of carbon monoxide and carbon dioxide are reduced to less than 5 ppm by the exothermic methanation reaction. [16,18].

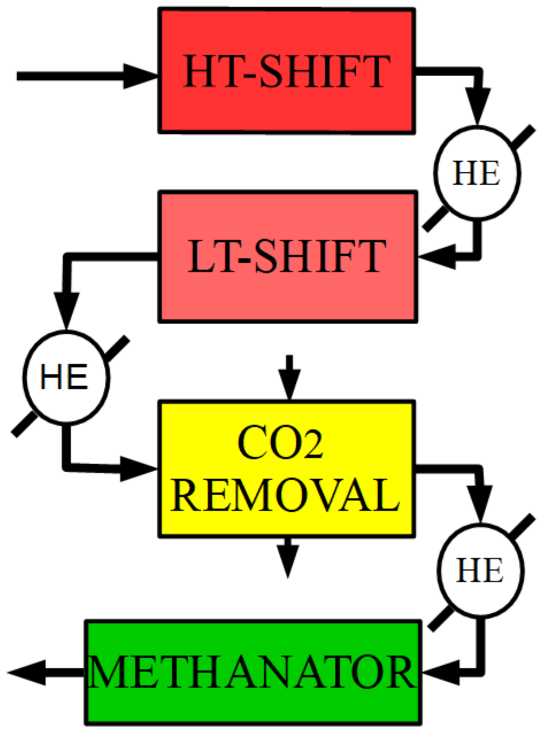

Figure 9: A schematic of all the simulated units in the Ammonia synthesis process.

5.2 Simulation in Aspen Plus

In this study, all three of the units just discussed where simulated using Aspen Plus and Aspen Plus Dynamics. A dynamic simulation is created using a steady-state simulation provided by Aspen [4]. Reaction rates for all reactions are implemented through FORTRAN code in Aspen plus using the compiling and linking functionality of the Aspen software. The reaction kinetics for all three units are as follows [4,9]:

High Temperature Shift Reaction: $CO + H_2O \rightleftarrows CO_2 + H_2$, $\Delta H = -41.2\ kJ/mol$:

$$r_{CO} = -A_c \exp\left(-\frac{300.69}{T} + 8.02\right) P^{\frac{1}{2}} \left(y_{CO} - \left(\frac{y_{H_2} y_{CO_2}}{K_{eq} y_{H_2O}}\right)\right), K_{eq} \exp\left(\frac{8240}{T} - 4.33\right) \quad (5)$$

Low Temperature Shift Reaction: $CO + H_2O \rightleftarrows CO_2 + H_2$, $\Delta H = -41.2\ kJ/mol$:

$$r_{CO} = -A_C \left(\frac{513.15}{T}\right) \left(\frac{\left(K_L y_{CO} y_{H_2O}^{\frac{1}{2}} \left(1 - \frac{K}{K_{eq}}\right)\right)}{\frac{1}{P} + K_A y_{CO} + K_B y_{CO_2}}\right), K = \left(\frac{y_{H_2} y_{CO_2}}{y_{CO} y_{H_2O}}\right)$$

$$K_{eq} = \exp\left(\frac{8240}{T} - 4.33\right), K_L = 68.4 \exp\left(-3620\left(\frac{1}{513.15} - \frac{1}{T}\right)\right)$$

$$K_A = 4.31 \exp\left(-4580\left(\frac{1}{513.15} - \frac{1}{T}\right)\right), K_B = 1.35 \exp\left(-1500\left(\frac{1}{513.15} - \frac{1}{T}\right)\right) \quad (6)$$

Methanation reaction 1: $CO + 3H_2 \rightleftarrows CH_4 + H_2O, \Delta H = -206\ kJ/mol$:

$$r_{CO} = -A_c 3.119 \exp\left(1300\left(\frac{1}{T} - \frac{1}{513}\right)\right)\left(\frac{P}{y_{H_2}}\right)^{\frac{1}{2}} \left(y_{CO} - \frac{y_{CH_4} y_{H_2O}}{y_{H_2}^3 P^2 \exp\left(-38.4523 + \frac{2627}{T}\right)}\right) \quad (7)$$

Methanation reaction 2: $CO_2 + 4H_2 \rightleftarrows CH_4 + 2H_2O, \Delta H - 164\ kJ/mol$:

$$r_{CO} = -A_c 3.119 \exp\left(1300\left(\frac{1}{T} - \frac{1}{513}\right)\right)\left(\frac{P}{y_{H_2}}\right)^{\frac{1}{2}} \left(y_{CO} - \frac{y_{CH_4} y_{H_2O}^2}{y_{H_2}^4 P^2 \exp\left(-38.4523 + \frac{2627}{T}\right)}\right) \quad (8)$$

Where r_{CO} is the reaction rate of CO in gmol/m^{3}s; A_C is the catalyst activity; T is the temperature in K; P is the total pressure in atm; and y_i is the mole fraction of component i.

All heat exchangers worked at fixed outlet temperature into each of their respective units. All tube reactors simulate are adiabatic. The adsorption column is simulated as a flash drum at

30ºC using ammonia to remove CO_2 and water. A detailed breakdown of the electrolyte solution chemistry and reaction kinetics in this adsorption column is discussed in Aspen Technology, Inc. (2017). Table 1 provides all the major parameters of each unit and their steady states.

Table 1: Parameter values of the ammonia process simulation.

	Parameter	Value
Feed	Temperature	980 $°C$
	Pressure	29 bar
	Mole flowrate	3435 mol/s
	Mole fraction y_{CO}	0.0839
	Mole fraction y_{CO_2}	0.0507
	Mole fraction y_{H_2}	0.355
	Mole fraction y_{H_2O}	0.353
	Mole fraction y_{N_2}	0.152
HT-shift	Reactor length	15.8 m
	Reactor diameter	4.4 m
	Loaded catalyst	9.61×10^4 kg
	Voidage	0.5
	Catalyst heat capacity	900 $J/kg\ K$
	Feed temperature	360 $°C$
LT-shift	Reactor length	7.7 m
	Reactor diameter	3.7 m
	Loaded catalyst	3.48×10^4 kg
	Voidage	0.5
	Catalyst heat capacity	850 $J/kg\ K$
	Feed temperature	210 $°C$
CO_2 Removal	Volume	49.09 m^3
	Temperature	30 $°C$
	Pressure	26.9 bar
	CO_2 remove rate	98.6 %
	H_2O remove rate	99.7 %
Methanator	Reactor length	4 m
	Reactor diameter	2.5 m
	Loaded catalyst	1.57×10^4 kg
	Voidage	0.5
	Catalyst heat capacity	900 $J/kg\ K$
	Feed temperature	280 $°C$

5.3 Disturbances

There are various disturbances that can occur in the ammonia synthesis process that can lead to unsafe conditions. It is possible that the catalytic activity in the first high temperature shift reactor decreases, leading to a decrease in the conversion of carbon monoxide. This will account for a great amount of carbon monoxide to reach the methanator. The excess CO in the methanator leads to more reaction during the exothermic methanation process, drastically increasing the temperature and potentially leading to thermal runaway.

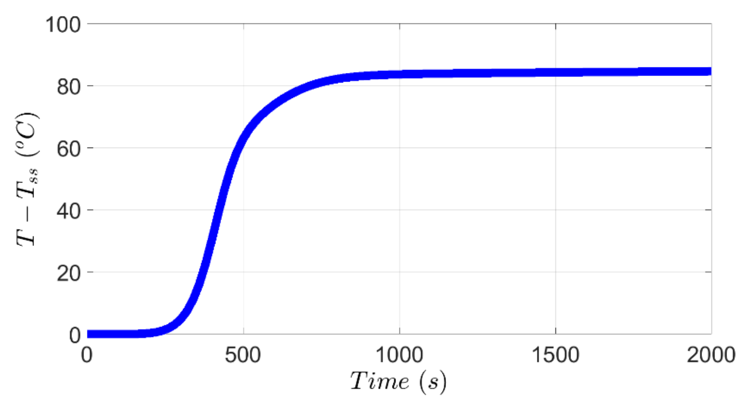

Figure 10: Methanator outlet temperature profile, showing that $T - T_{ss}$ increases more than 80ºC after decreasing catalyst activity from 1 to 0.1 over 300s

Another possible occurrence involves the decrease in temperature of the feed entering the first high temperature shift reactor. As the process must take place at high temperature, a lower temperature will lead to less CO reaction in the shift reactor. This extra CO will once again cause an increase in reactivity in the highly exothermic methanation unit. Thus, we will focus on designing a controller that controls outlet methanation temperature by manipulating the methanator inlet feed temperature.

Chapter 6

Safeness Index-based Model Predictive Controller: Case Study 2

6.1 Model Identification

The methanator is simulated at the steady-state feed temperature T_{in}= 280ºC and outlet temperature T_{out}=327.27ºC. The primary cause of disturbance in these simulations will be the concentration of CO in the feed, having a steady-state mole fraction value of $3.55x10^{-3}$. For our simulation the state, input, and disturbance deviation variables will be $x = T_{out} - T_{out}^{ss}$, $u = T_{in} - T_{in}^{ss}$ and $d = y_{CO} - y_{CO}^{ss}$ so that the point of equilibrium is set at zero. As there is a time delay between the feed temperature and the outlet temperature, we will be utilizing a linear dynamic model with time delay. Just as we did before, transient response data is generated from our simulation using a step change in feed temperature. Using the generated data and a MOSEP algorithm in MATLAB to identify the matrices A and B of our linear model. Another simulated step change in CO mole fraction is used to calculate the gain in K of the disturbance d. Our linear dynamic model takes the following form.

$$\frac{dx(t)}{dt} = Ax(t) + Bu(t - t_d) + Kd(t - t_d) \tag{9}$$

$$A = -.005136; \quad B = 0.01207; \quad K = 32.887; \quad t_d = 100s$$

6.2 Safeness Index-based MPC Design

As the disturbances in this case study have a huge effect on the outlet temperature of the Methanation unit, high outlet temperatures will be our unsafe operating conditions. All temperatures under the steady-state temperatures will be considered safe conditions. Thus, our Safeness Index takes on the form

$$S(x) = [f^{+}(x)]^{2} \tag{10}$$

Where f^+ is the same function in equation 2. The quadradic form will once again give significantly large weight to temperatures T_{out} that are far above the steady state. A conservative Safeness Index Threshold should be considered when taking into account model mismatch, sample-and-hold controller, and the time delay in our dynamic model. The index threshold is chosen to be $S_{TH} = 25$, allowing for only a 5º change. This is conservative considering we saw that the outlet feed temperature can increase by even 80ºC. We will also incorporate MPC with a feedforward control action.

$$u(t_k) = u_{MPC}(t_k) + u_{forward}(t_k) \tag{11}$$

This means that the control action $u(t_k)$ consists of a feedforward term calculated by equation 12 and $u_{MPC}(t_k)$ is the first control action in the solution $u^{*}(t)$ to the optimization problem of equation 13.

$$u_{forward}(t_k) = -\frac{K}{B} d(t_k) \tag{12}$$

$$\min_{u\in S(\Delta),y} \int_{t_k}^{t_{k+N}+t_d} \|\tilde{x}(\tau)\|_{Q_c}^2 + \int_{t_k}^{t_{k+N}} \|u(\tau)\|_{R_C}^2 \, d\tau + \sum_{i=1}^{N} k_1 e^{-k_2 y(i)}, k_1, k_2 > 0 \tag{13a}$$

$$\text{s.t} \qquad \dot{\tilde{x}}(t) = A\tilde{x}(t) + Bu(t - t_d) \tag{13b}$$

$$\tilde{x}(t_k) = x(t_k) \tag{13c}$$

$$u(t) = u_{pre}(t), \forall t \in [t_k - t_d, t_k] \tag{13d}$$

$$u(t) \in U, \forall t \in [t_k, t_{k+N}] \tag{13e}$$

$$S(\tilde{x}(t_k + i)) + y(i) \le S_{TH},\ i = 1,2, \dots, N \tag{13f}$$

$$y(i) \in R,\ i = 1,2, \dots, N, \quad if\ S(x(t_k)) > S_{TH} \tag{13g}$$

$$y(i) \ge 0,\ i = 1,2, \dots, N, \quad if\ S(x(t_k)) \le S_{TH} \tag{13h}$$

Here the notation of the optimization problem follows the same notation as equation 4. Equation (13a) is minimizing the integral term and the penalty term of slack variable $y(i)$. The constraint (13b) is the nominal linear model used to predict the states of the closed-loop system. Equation (13c) is the initial condition $\tilde{x}(t_k)$ of the optimization problem evaluated at $t = t_k$. Equation (13d) uses input trajectories calculated from previous steps to predict states from t_k to $t_k + t_d$. Equation (13e) is the input constraint over the entire prediction horizon, the manipulated input $180°\text{C} \le T_{in} \le 380°\text{C}$. Equation 13 is the Safeness index constraint with slack variable $y(i)$. The soft constraint allows for a gradual change in input as the index gets close to the threshold. When the index is below the threshold, nonnegative slack variables ensure that the constraint (4e) holds. And when the index is above the threshold, negative slack variable ensure that the constraint (4e) still holds. The parameters k_1 and k_2 should be chosen carefully such that the slack variables have little effect through the penalty term in equation (4a) when below the threshold and significant effect when above the threshold. For this case study parameters k_1 and k_2 are 10^5 and .2 respectively.

The optimization problem of the Safeness Index-based MPC of equation 13 was solved using the solver FilterSD on OPTI Toolbox in MATLAB; sampling period 20s and prediction horizon N = 30. Then explicit Euler was used to integrate the dynamic model; step size 10^{-1}.

Chapter 7

Simulation Results: Case Study 2

7.1 Disturbance: Catalyst Activity

The disturbance that is introduced is the decreases of catalyst activity in the high temperature shift reactor from 1 to 0.1 over the span of 300 seconds. This decrease in activity leads to the higher concentration of CO that reaches the methanator, leading to an increase in temperature. When there is a decrease in catalytic activity, there are possibly other disturbances that also maybe be contributing to the increase in temperature; an example would be excess carbon dioxide. With all these other factors, model mismatch exists between the identified linear model and the actual process. Even though, the Safeness Index Based MPC can mitigate some of the temperature increases, it is not able to bring the system back to the origin.

In this study we compared the ability of the MPC controller to control the increases in temperature with and without a safeness index. We can see in the figure that without the safeness index the outlet temperature of the methanator can reach about 30ºC. When incorporating a safeness index the temperature can exit at a lower temperature, which is desirable. It was shown that though the Safeness Index Based MPC can not return the system to the origin, it can possibly improve process operation safety of the ammonia plant.

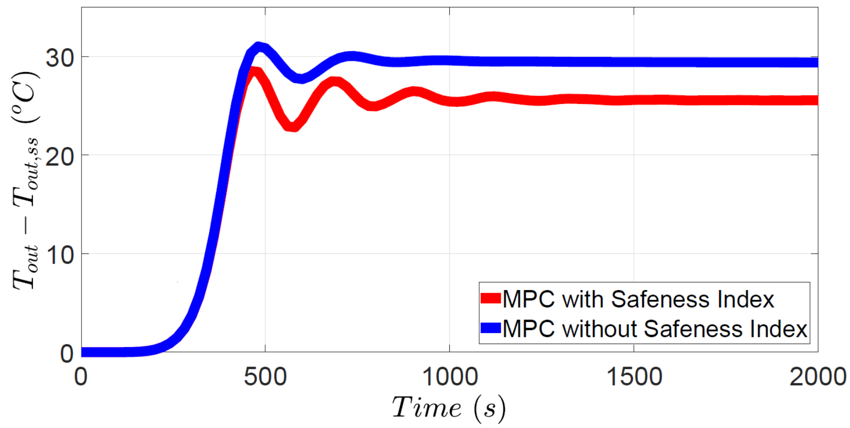

Figure 11: Methanator outlet temperature, showing that MPC with Safeness Index guides system to lower temperature.

Chapter 8

Conclusion

The focus of this work was to test for improvements in process operational safety by employing a Safeness Index-based Model Predictive Controller. We implemented a Safeness Index-based MPC onto two safety critical chemical processes. In the first study, we simulated a high-pressure flash drum in tandem with a pressure relief valve and analyzed the advantages of incorporating a Safeness Index in the model predictive control. A Safeness Index and Safeness Index threshold were designed using information from the process and the safety system already employed. Using both Aspen and MATLAB, a dynamic linear model was identified and integrated forward in time with our MPC. This allowed us to explore how the system and the MPC mitigated varying disturbance sizes. It was demonstrated that when introduced to small disturbances, the flash drum stays below the opening pressure of the relief valve. However, when introduced to a large disturbance the controller was not able to avoid activating the relief valve. Once the relief valve closed, the MPC was able to return the system back to its steady state.

In the second case study, four units of the ammonia synthesis process were simulated and a Safeness Index MPC was applied. A safeness index function, threshold and dynamic linear model was once again developed considering delay. Though the controller was not able to return the system to the original steady state, it demonstrated that using a Safeness Index can guide the system to safer conditions.

Bibliography

[1] Albalawi, F., Alanqar, A., Durand, H. Christofides. P.D., 2016. A feedback control framework for safe and economically-optimal operation of nonlinear processes. AIChE Journal 62, 2391-2409

[2] Albalawi, F., Durand, H., Christofides, P.D., 2017. Process operational safety using model predictive control based on a process safeness index. Computers & Chemical Engineering 104, 76-88.

[3] Appl, M., 2000 Ammonia/ Ullmann's Encyclopedia of Industrial Chemistry.

[4] Aspen Technology, Inc., 2017. Aspen Plus ammonia model. Bedford, MA.

[5] Bø, T.I., Johansen, T.A., 2014. Dynamic safety constraints by scenario based economic model predictive control, in: Proceedings of the IFAC World Congress, Cape Town, South Africa. pp. 9412-9418

[6] Center for Chemical Process Safety, 2008. Guidelines for Hazard Evaluation Procedures. Third ed., John Wiley and Sons, Inc., Hoboken, New Jersey.

[7] Ellis, M., Durand, H., Christofides, P.D., 2014. A tutorial review of economic model predictive control methods. Journal of Process Control 24, 1156-1178.

[8] Ellis, m., Liu, j., Christofides, P.D., 2016. Economic Model Predictive Control: Theory, Formulations and Chemical Process Applications. Springer, London, England.

[9] Ettouney, H.M., Shaban, H.I., Nayfeh, L.J., 1995. Theoretical analysis of high and low temperature shift converters. Chemical Engineering Communications 134, 1-16.

[10] Gonzales, D., Gulden, T.R., Strong, A., Hoyle, W., 2016. Cost-benefit Analysis of Proposed California Oil and Gas Refinery Regulations. Rand Corporation.

[11] Lao, L., Ellis, M., Christofides, P.D., 2013. Proactive fault tolerant model predictive control. AIChE Journal 59, 2810-2820.

[12] Leveson, N.G., Stephanopoulos, G., 2014. A system-theoretic, control-inspired view and approach to process safety. AICheE Journal 60, 2-14.

[13] Marsh & McLennan Companies Inc, 2016. The 100 Largest Losses 1974-2015: Large Property Damage Losses in the Hydrocarbon Industry. Technical report. March & McLennan Companies Inc.

[14] Mayne, D.Q., Rawlings, J.B., Rao, C.V., Scokaert, P.O.M., 200. Constrained model predictive control: Stability and optimality. Automatica 36, 789-814.

[15] Mhaskar, P., Liu, J., Christofides, P.D., 2013. Fault-Tolerant Process Control: Methods and Applications. Springer-Verlag, London, England.

[16] Ojha, M., Dhiman, A.K., 2010. Problem, failure and safety analysis of ammonia plant: a review. International Review of Chemical Engineering 2, 631-646.

[17] Rawlings, J.B., 2000. Tutorial overview of model predictive control. IEEE Control Systems Magazine 20, 38-52.

[18] Twigg, M., 1989. Catalyst handbook. Wolfe Publishing Ltd., London.

[19] Wu, Z., Albalawi, F., Zhang, Z., Zhang, J., Durand, H., Christofides, P.D., 2018a. Model predictive control for process operational safety: Utilizing safeness index-based constraints and control Lyapunov-barrier functions. Computer Aided Chemical Engineering 44, 505-510.

[20] Wu, Z., Durand. H., Christofides, P.D., 2018b. Safeness index-based economic model predictive control of stochastic nonlinear systems. Mathematics 6, 69.

[21] Zhang, Z., Wu, Z., Durand, H., Albalawi, F., Christofides, P.D., 2018. On integration of feedback control and safety systems: Analyzing two chemical process applications. Chemical Engineering Research and Design 132, 616-626.