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Master Thesis

Application of Sontag's Universal Stabilizer to the Continuous Stirred Tank Reactor

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Abstract

The design of a controller for the continuous stirred tank reactor (CSTR) has been widely studied. Currently, conventional control methods based on operating point linearization which guarantee good performance in a suitable neighborhood of the operating point are mainly used. Nonlinear control laws suggest a larger range of good performance, if we are considering the system in the neighborhood of the equilibrium point, and it is mainly based on the input-output linearization methods. Regarding the nonlinear control laws, several approaches to modern feedback design start with a control Lyapunov function (clf) for a system, and use this function in order to construct a stabilizing feedback.

In this thesis, the open loop behavior of a CSTR model is firstly studied. By observing the fact that system is unstable, the feedback design is taken into consideration. This has been done by implementing the Sontag's stabilizer which is a consequence of Sontag's theorem on nonlinear stabilization. This theorem states that the existence of a smooth clf implies smooth stabilizability [8]. We have considered the classical quadratic form as a Lyapunov functional. It is qualitatively shown that the constructed feedback parameters satisfy the necessary condition to prove that the suggested quadratic form is indeed clf.

The first two chapters introduce the structural design of chemical reactors, and specifically CSTR reactors. Moreover, in Chapter 2, the set of governing nonlinear ODEs corresponding to the jacket cooled CSTR is obtained. The open loop behavior is briefly discussed in Chapter 3 and it is followed by the theoretic argument about the Sontag's theorem and feedback design. Finally, in the last two chapters we explained the implemented program in Matlab and the simulation result is depicted. This thesis is finished by a short note on the possible future development regarding this research.

Chapter 1

Reactor Basics

In this chapter we first review some of the basics of chemical equilibrium and reaction kinetics. We need to understand clearly the fundamentals about chemical reaction rates and chemical equilibrium, particularly the effects of temperature on rate and equilibrium for different types of reactions. Reactions are generally categorized as exothermic (releasing energy) or endothermic (requiring energy), as reversible (balance of reactants and products) or irreversible (proceeding completely to products), and as homogeneous (single-phase) or heterogeneous (multiphase). Subsequently, we will extensively discuss the reaction type which has been studied in this thesis with more details. Next, there will be a brief review on the different types of chemical reactors including Continues Stirred Tank Reactor (CSTR).

1.1 FUNDAMENTALS OF KINETICS AND REACTION EQUILIBRIUM

The reaction rate (rate of reaction) or speed of reaction for a reactant or product in a particular homogenous system is intuitively defined as how fast or slow a reaction takes place. For example, the oxidative rusting of iron under Earth's atmosphere is a slow reaction that can take many years, but the combustion of cellulose in a fire is a reaction that takes place in fractions of a second. Chemical kinetics is the part of physical chemistry that studies reaction rates. The rate at which a chemical reaction occurs depends primarily on temperature and the concentrations of reactants and products [1]. Other variables, such as pressure and reaction order could be also influencing the reaction rate, but usually it happens in a lower extent. It might be helpful to have a brief review of how the mentioned parameters influence a reaction.

- Temperature: Usually conducting a reaction at a higher temperature delivers more energy into the system and increases the reaction rate by causing more collisions between particles, as explained by collision theory. However, the main reason that temperature increases the rate of reaction is that more of the colliding particles will have the necessary activation energy resulting in more successful collisions (when bonds are formed between reactants).

- Concentration: Reaction rate increases with concentration, as described by the rate law and explained by collision theory. As reactant concentration increases, the frequency of collision increases.

- Pressure: The rate of gaseous reactions increases with pressure, which is, in fact, equivalent to an increase in concentration of the gas. The reaction rate increases in the direction where there are fewer moles of gas and decreases in the reverse direction. For condensed-phase reactions, the pressure dependence is weak.

- Order: The order of the reaction controls how the reactant concentration (or pressure) affects reaction rate.

In heterogeneous systems, chemical reaction rates can become more complex because they may not be governed solely by chemical kinetics but also by the rate of mass and/or heat transfer, which often play significant roles.

1.2 POWER LAW KINETICS

If we consider the irreversible reaction with two reactants forming a product the overall rate of reaction K can be viewed as the moles of component A being consumed per unit time per unit volume.

$$\mathrm{A} + \mathrm{B} \rightarrow \mathrm{C} \quad (1.1)$$

Sometimes reaction rates are based per mass of catalyst present. Of course, by stoichiometry in this system, the moles of component B consumed have to equal the moles of A, along with the moles of component C produced. The chemical reaction rate law is essentially an algebraic equation involving concentration, not a differential equation [2]. For example, the algebraic form of the rate law for mentioned reaction may be a function of concentrations,

$$\mathrm{K} = \mathrm{k(T)}\ \mathrm{C}_\mathrm{A}^{\alpha}\ \mathrm{C}_\mathrm{B}^{\beta} \quad (1.2)$$

The exponents α and β are reaction orders for the respective two reactants. The actual reaction mechanism determines the form of the kinetic expression. For a given reaction, the particular concentration dependence that the rate law follows (i.e. $\mathrm{k(T)}\ \mathrm{C}_\mathrm{A}^{1}\ \mathrm{C}_\mathrm{B}^{1}$, $\mathrm{k(T)}\ \mathrm{C}_\mathrm{A}^{2}\ \mathrm{C}_\mathrm{B}^{2}$ or …) must be determined from experimental observation [2]. Each reaction rate coefficient k has a temperature dependency, which is usually given by the Arrhenius equation:

$$\mathrm{k} = \mathrm{k}_0 \mathrm{e}^{\frac{-\mathrm{E}}{\mathrm{RT}}} \quad (1.3)$$

E is the activation energy and R is the gas constant. Since at temperature T the molecules have energies given by a Boltzmann distribution, one can expect the number of collisions with energy greater than E to be proportional to $\mathrm{e}^{\frac{-\mathrm{E}}{\mathrm{RT}}}$. k_0 is the pre-exponential factor or frequency factor. The k_0 pre-exponential factor is a large positive number (much greater than one) and has unit that depends on the concentration units and the order of the reaction with respect to each component. The exponential term in Eq. (1.3) is a small positive number. Its minimum value is zero (when $\frac{E}{RT}$ is infinite at very low absolute temperatures because of the negative sign in the exponential). Its maximum value is unity (when $\frac{E}{RT}$ is zero at very high temperatures). Therefore at low temperature the $\frac{E}{RT}$ term becomes large, which makes the exponential small and produces a low specific reaction rate. Conversely, at high temperature the $\frac{E}{RT}$ term becomes small, which makes the exponential approach unity (in the limit as temperature goes to infinity, the exponential term goes to one). Thus the specific reaction rate increases with increasing temperature [1]. Clearly the rate of change of $k(T)$ with temperature depends on the value of the activation energy. Figure 1.1 compares the relative rates of reaction as a function of activation energy and temperature.

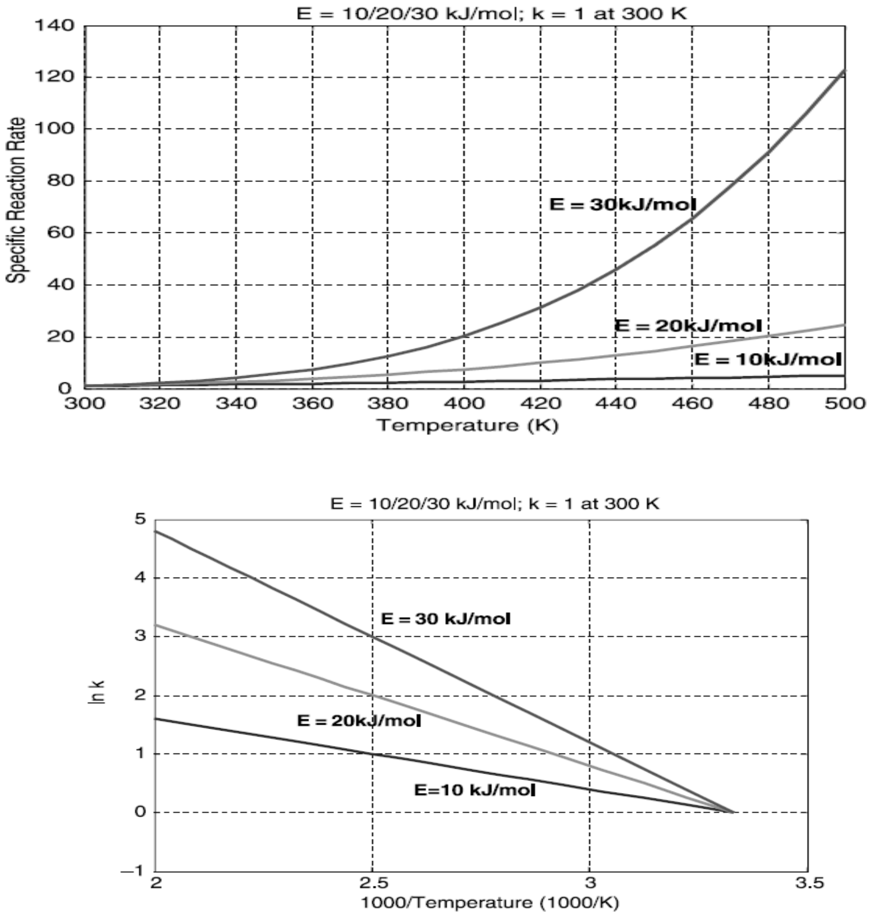


Figure 1.1: Effect of activation energy on temperature dependence of reaction rate.

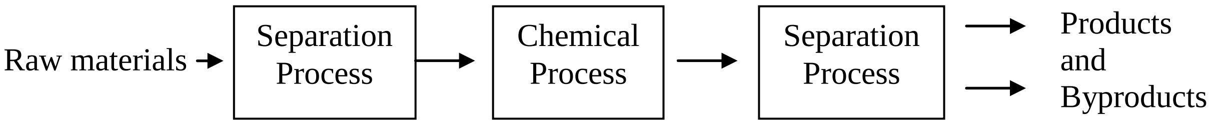
The activation energies are 10, 20, and 30 $\frac{kj}{mol}$, and the reaction rates are calculated relative to a rate of unity at 300 K. Reactions with low activation energies are relatively insensitive to temperature, whereas reactions with high activation energies are quite sensitive to temperature. This can be seen by comparing the slopes of the lines for the relative reaction rates versus $\frac{1}{\mathrm{T}}$. With activation energy of $10\frac{\mathrm{kj}}{\mathrm{mol}}$, the change in reaction rate from 300 to 500 K is much less than the change at activation energy of $30\frac{\mathrm{kj}}{\mathrm{mol}}$. Also, we see that the sensitivity of reaction rate to temperature is relatively greater at lower than at higher temperatures. Both of these observations play a role in the control of temperature in a chemical reactor. The main point of the discussion above is that the specific reaction rates always increase as temperature increases and the higher the activation energy, the more sensitive the reaction rate is to temperature.

1.3 DETERMINING KINETIC PARAMETERS

The many pre-exponential factors, activation energies and reaction order parameters required to describe the kinetics of chemical reactors must be determined, usually from laboratory, pilot plant, or plant experimental data. Ideally, the chemist or biologist has made extensive experiments in the laboratory at different temperatures, residence times and reactant concentrations. From these data, parameters can be estimated using a variety of mathematical methods. Some of these methods are quite simple. Others involve elegant statistical methods to attack this nonlinear optimization problem. A discussion of these methods is beyond the scope of this thesis. The reader is referred to the textbooks. In many practical applications, the engineer often has only plant performance data to use to back-calculate kinetic parameters. Data of this type are seldom extensive enough to permit precise calculation of all parameters since the plant normally operates in a fairly narrow window of operating conditions. However, useful simplified kinetics and parameters can often be determined that describe the major kinetics inside this region. Extrapolation outside the region from which the data has been obtained is very risky [1].

1.4 TYPES AND FUNDAMENTAL PROPERTIES OF REACTORS

The chemical reactor is the heart of any chemical process. Chemical processes turn inexpensive chemicals into valuable ones, and chemical engineers are the only people technically trained to understand and handle them. While separation units are usually the largest components of a chemical process, their purpose is to purify raw materials before they enter the chemical reactor and to purify products after they leave the reactor. Here is a very generic flow diagram of a chemical process.



Raw materials from another chemical process or purchased externally must usually be purified to a suitable composition for the reactor to handle. After leaving the reactor, the unconverted reactants, any solvents, and all byproducts must be separated from the desired product before it is sold or used as a reactant in another chemical process. The key component in any process is the chemical reactor; if it can handle impure raw materials or not produce impurities in the product, the savings in a process can be far greater than if we simply build better separation units. In typical chemical processes the capital and operating costs of the reactor may be only 10 to 25% of the total, with separation units dominating the size and cost of the process. Yet the performance of the chemical reactor totally controls the costs and modes of operation of these expensive separation units, and thus the chemical reactor largely controls the overall economics of most processes. Improvements in the reactor usually have enormous impact on upstream and downstream separation processes [3].

Figure1.2: Typical Chemical Reactors

Reactors can be operated in batch (no mass flow into or out of the reactor) or flow modes. Flow reactors operate between limits of completely unmixed contents (the plug-flow tubular reactor or PFTR) and completely mixed contents (the continuous stirred tank reactor or CSTR) [1].

In the next chapter, we are going to study the CSTR reactors in details, since this system has been studied to be stabilized using Sontag's universal stabilizer in the later chapters.

Chapter 2

Continuous Stirred Tank Reactor

The continuous flow stirred-tank reactor (CSTR), also known as back-mix reactor, is a common ideal reactor type in chemical engineering. A CSTR often refers to a model used to estimate the key unit operation variables when using a continuous agitated-tank reactor to reach a specified output. The mathematical model works for all fluids: liquids, gases, and slurries. The behavior of a CSTR is often approximated or modeled by that of a Continuous Ideally Stirred-Tank Reactor (CISTR). All calculations performed with CISTRs assume perfect mixing. In a perfectly mixed reactor, the output composition is identical to composition of the material inside the reactor, which is a function of residence time and rate of reaction. If the residence time is 5-10 times the mixing time, this approximation is valid for engineering purposes. The CISTR model is often used to simplify engineering calculations and can be used to describe research reactors. In practice it can only be approached, in particular in industrial size reactors.

2.1 FUNDAMENTALS

Figure 2.1 shows a vessel with an agitator for mixing, a jacket that surrounds the vessel for heating or cooling, feed lines entering the vessel and a liquid product stream exiting from the bottom. The liquid in the reactor is assumed to be perfectly mixed, that is, with no radial, axial, or angular gradients in properties (temperature and composition). The product stream has a composition and a temperature that are exactly the same as the contents of the liquid throughout the vessel. This is always true, both under steady-state conditions and dynamically at any point in time.

This characteristic of a CSTR immediately generates an inherent weakness of the CSTR type of reactor, that is, the concentration of reactant in the vessel is the same as the concentration of reactant in the product. The concentration of reactant is inversely related to conversion. Fractional conversion χ defined as

$$\chi = \frac{C_{A0} - C_A}{C_{A0}} \qquad (2.1)$$

If a high conversion is desired, the reactant concentration must be small. But the reaction rate depends directly on the reactant concentration. It also depends on the reactor volume. So, if a high conversion desired, the reactor must be large to compensate for the small reactant concentration. Thus a single CSTR is seldom used if high conversion is desired. Of course, using several CSTRs in series is one way to reduce the total reactor volume because only the last vessel will have the small reactant concentration [1].

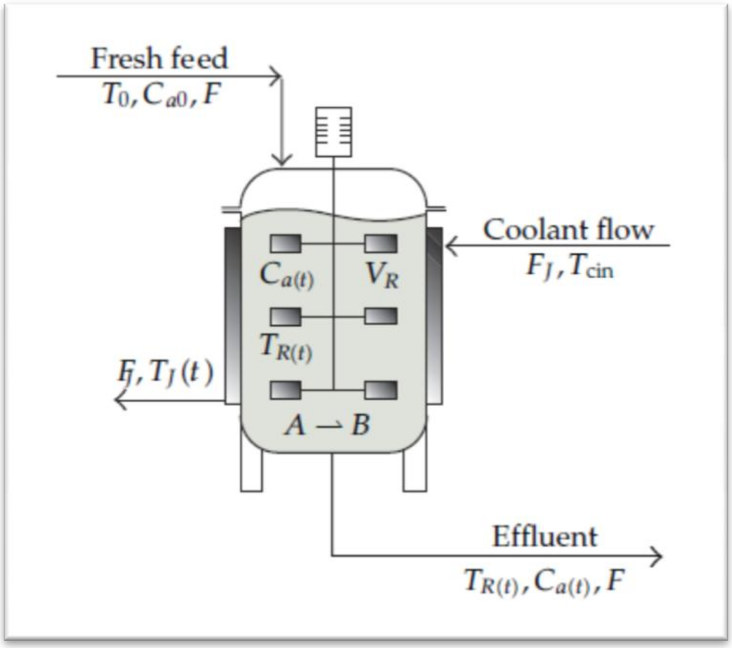


Figure 2.1: Schematic CSTR with jacket.

We will develop detailed steady-state and dynamic mathematical models of CSTRs in the next chapters with and irreversible exothermic single phase reaction. For the moment, let us just make some qualitative observations. There are several features of a CSTR that impact controllability:

- A variety of methods and configurations can be used for heat transfer. Since heat transfer is one of the key issues in reactor control, the CSTR is usually more easily controlled than the other reactor types.

- The temperature of the feed has some effect on controllability, but it is much less important in a CSTR than in a tubular reactor, if heat is being removed from the reactor, a feed that is at a lower temperature than the temperature in the reactor will reduce the heat transfer requirements.

- Conversion is the fraction of a reactant that is fed to the reactor that reacts in the reactor. The level of conversion in a CSTR has a very significant impact on its stability and controllability. A high conversion means a small reactant concentration in the reactor vessel, so there is little “fuel” available to permit a reactor runaway. On the other hand, a low conversion means that there is plenty of reactant available to react. If the reaction is exothermic and irreversible, a reactor temperature runaway can more easily occur in a

CSTR operating with low reactant conversion than in one operating with high reactant conversion. In addition to affecting reactant concentration, the design conversion affects reactor size. Low conversion means a smaller reactor. This small reactor has less heat transfer area if an external jacket or an internal coil is used, which has a negative impact on controllability.

2.2 FIRST ORDER IRREVERSIBLE EXOTHERMIC REACTION

The type of reaction which has been taken to consideration for studying controllability in this thesis is the first order irreversible exothermic reaction. Prior to stating the CSTR model formulation it is necessary to have a quick review on the terms which define the reaction type.

2.2.1 First Order Reaction:

Consider the reaction (2.2) Where A is converted to B.

$$A \rightarrow B \qquad (2.2)$$

$$v = -\frac{d[A]}{dt} = \frac{d[B]}{dt} = -k[A]^1 \qquad (2.3)$$

Eq. (2.3), which defines the algebraic relation between reaction velocity and concentration, is called the rate law for the reaction. The exponent in the above equation in the term $[A]^1$ means that the rate depends upon the concentration of the reactant [A] raised to the first power; i.e. it means that if the concentration of A is doubled, the rate also doubles.

2.2.2 Irreversible Reaction:

Chemical reactions which proceed to completion in one direction only are known as irreversible reactions. In irreversible reactions reactants are completely converted into products in a certain interval of time. In these reactions products do not form reactants again.

2.2.3 Exothermic Reaction:

An exothermic reaction is a chemical or physical reaction that releases heat. It gives out energy to its surroundings. The energy needed for the reaction to occur is less than the total energy released.

2.3 MASS, COMPONENT AND ENERGY BALANCE

The fundamental balance equations resulting to the CSTR model for a first order irreversible exothermic reaction can be summarized in mass and energy balance equations. It might be helpful to have a quick look at the definition of these equations, before proceeding to formulating the CSTR model.

2.3.1 Mass Balance:

A mass balance, also called a material balance, is an application of conservation of mass to the analysis of physical systems. By accounting for material entering and leaving a system, mass flows can be identified which might have been unknown, or difficult to measure without this technique. The exact conservation law used in the analysis of the system depends on the context of the problem, but all revolve around mass conservation, i.e. that matter cannot disappear or be created spontaneously.

2.3.2 Energy Balance:

We can keep track of the movement of energy and changes in its form using energy balances, which are analogous to the mass balances we discussed in the previous section. We can do this because of the law of conservation of energy which states that energy can neither be produced nor destroyed. As long as we consider all the possible forms of energy, there is no term in energy balances which is analogous to the chemical reaction term in mass balances. That is, we can treat energy as a conservative substance

Now we are well-equipped to introduce the Steady State CSTR model for a first order irreversible exothermic reaction. In the coming subsections the approach of deriving steady state and nonlinear dynamic model corresponds to the ones which have been developed in [1] and [4].

2.4 STEADY STATE MODEL

2.4.1 CSTR without Jacket

In this section we study the steady-state design of perfectly mixed, continuously operating, liquid phase reactors. Consider the first order irreversible reaction (2.2) as explained in the first chapter the reaction rate K is

$$K = k\, C_A = C_A\, k_0 e^{\frac{-E}{RT_R}} \qquad (2.4)$$

Where

K = by considering (2.3) is the consumption rate of reactant A ($\mathrm{kmol\ s^{-1} m^{-3}}$)

k = specific reaction rate (s^{-1})
C_A= concentration of reactant A in reactor ($\frac{kmol}{m^3}$)
k_0= pre-exponential factor (s^{-1})
E = Activation energy ($\frac{J}{kmol}$)
R = 8314 ($J\ kmol^{-1}\ K^{-1}$)
T_R = reactor temperature (K)

As previously mentioned, the reactor steady state is described by three algebraic balances: a total mass balance, a component balance (since there are only two components), and an energy balance:

Total mass balance:

$$\rho_0\, F_0 = \rho\, F \qquad (2.5)$$

Component A balance:

$$F_0 C_{A0} = F\, C_A + V_R\, K = F\, C_A + V_R\, k\, C_A \qquad (2.6)$$

Reactor energy balance:

$$\rho_0\, c_{p0}\, F_0\, T_0 = \rho\, c_p\, F\, T_R + \lambda\, V_R K + Q \qquad (2.7)$$

Where

ρ_0 = density of feed stream ($\frac{kg}{m^3}$)
F_0 = rate of the feed flow ($\frac{m^3}{s}$)
ρ = density of product stream ($\frac{kg}{m^3}$)
F = rate of product flow ($\frac{m^3}{s}$)
C_{A0} = concentration of reactant A in the feed ($\frac{kmol}{m^3}$)
V_R = volumetric holdup of liquid in reactor (m^3)
T_0 = temperature of the feed (K)
c_p = heat capacity of feed ($J\ kg^{-1}\ K^{-1}$)
λ = heat of the reaction ($\frac{J}{kmol}$)
Q = rate of heat removal from liquid in reactor ($\frac{J}{s}$)

2.4.2 Jacket Cooled CSTR

The Q term in Eq. (2.7) depends on the heat removal scheme used. If a circulating jacket water system is used, the jacket is essentially at one temperature T_J, and the heat transfer rate depends on the jacket area, the overall heat transfer coefficient and the differential temperature driving force

$$Q = U A_J (T_R - T_J) \quad (2.8)$$

Where

U = overall heat transfer coefficient ($W K^{-1} m^{-2}$)
A_J= jacket heat transfer area (m^2) = π D L
D = reactor diameter (m)
L = reactor length (m)

The consumption of the cooling medium is calculated from an energy balance around the perfectly mixed jacket at temperature T_J. Constant physical properties of the cooling medium are assumed

$$F_J \rho_J c_J T_{C,in} = F_J \rho_J c_J T_J - Q \quad (2.9)$$

Where

ρ_J = density of coolant ($\frac{kg}{m^3}$)
F_J = rate of the coolant flow ($\frac{m^3}{s}$)
c_p= heat capacity of coolant ($J kg^{-1} K^{-1}$)
$T_{C,in}$= supply temperature of cooling medium (K)

The conversion χ of reactant A is given by

$$\chi = \frac{C_{A0} - C_A}{C_{A0}} \quad (2.10)$$

2.5 NONLINEAR DYNAMIC MODEL

In this subchapter we derive the nonlinear dynamics of jacket cooled CSTR model by referring to [1] and [5]. In the coming chapters regarding this dynamical system, we will discuss the open loop control law and the feedback control design of the system using Sontag's theory.

By recalling the reaction (2.2), the dynamic model of the reactor and jacket consists of four nonlinear ordinary differential equations:

Total mass balance:

$$\frac{d(V_R\,\rho)}{dt} = \rho_0\,F_0 - \rho\,F \quad (2.11)$$

Component A balance:

$$\frac{d(V_R\,C_A)}{dt} = F_0 C_{A0} - F\,C_A - V_R\,K = F_0 C_{A0} - F\,C_A - V_R\,k\,C_A \quad (2.12)$$

Reactor energy balance:

$$\frac{d(V_R\,\rho\,c_p\,T_R)}{dt} = \rho_0\,c_{p0}\,F_0\,T_0 - \rho\,c_p\,F\,T_R - \lambda\,V_R K - Q \quad (2.13)$$

Where

ρ_0 = density of feed stream ($\frac{kg}{m^3}$)
F_0 = rate of the feed flow ($\frac{m^3}{s}$)
ρ = density of product stream ($\frac{kg}{m^3}$)
F = rate of product flow ($\frac{m^3}{s}$)
C_{A0} = concentration of reactant A in the feed ($\frac{kmol}{m^3}$)
V_R = volumetric holdup of liquid in reactor (m^3)
T_0 = temperature of the feed (K)
c_p = heat capacity of feed ($J\,kg^{-1}\,K^{-1}$)
λ = heat of the reaction ($\frac{J}{kmol}$)
Q = rate of heat removal from liquid in reactor ($\frac{J}{s}$)

Note that the heat of reaction λ is negative for exothermic reactions, so the third term on the right-hand side of Eq. (2.13) is positive. This means that an increase in the reaction rate tends to increase the reactor temperature. With a circulating jacket water system with a jacket temperature T_J, the heat transfer rate depends on the jacket area, the overall heat transfer coefficient, and by considering the differential temperature driving force, Eq. (2.8), the CSTR dynamical model can be expressed by the following ordinary differential equations:

The dynamical model of the jacket is:

$$\frac{d(V_J\,\rho_J\,c_J\;T_J)}{dt} = F_J\,\rho_J\,c_J\,T_{C,in} - F_J\,\rho_J\,c_J\,T_J + Q \qquad (2.14)$$

Where

F_J = rate of the coolant flow ($\frac{m^3}{s}$)
ρ_J = density of coolant ($\frac{kg}{m^3}$)
c_J = heat capacity of coolant ($J\,kg^{-1}\,K^{-1}$)
$T_{C,in}$ = supply temperature of the coolant medium (K)

If physical properties are assumed constant (densities and heat capacities), these terms can be pulled outside the time derivatives in Eqs. (2.11) to (2.14). If reactor volume is held constant (by a level controller) and the jacket volume is constant, the V_R and V_J terms can also be taken out of the derivatives. Equation (2.11) reduces to

$$F_0 = F \qquad (2.15)$$

And the other three differential equations reduce to the following set:

$$\frac{dC_A}{dt} = \frac{F}{V_R}(C_{A0} - C_A) - C_A\,k_0 e^{\frac{-E}{RT_R}} \qquad (2.16)$$

$$\frac{dT_R}{dt} = \frac{F}{V_R}(T_0 - T_R) - \frac{\lambda\,C_A\,k_0 e^{\frac{-E}{R\,T_R}}}{\rho\,c_p} - \frac{U\,A_J\,(T_R - T_J)}{V_R\,\rho\,c_p} \qquad (2.17)$$

$$\frac{dT_J}{dt} = \frac{F_J}{V_J}\left(T_{C,in} - T_J\right) + \frac{U\,A_J\,(T_R - T_J)}{V_J\,\rho_J\,c_J} \qquad (2.18)$$

In the next chapters, these three nonlinear ordinary differential equations will be used to simulate the dynamic performance of the CSTR. The open loop behavior applies when no controllers are used. In this case the flow rate of the cooling water (F_J) is held constant. With closed loop behavior, a temperature controller is installed that manipulates cooling water flow to maintain reactor temperature. The controlling input signal will be generated by applying Sontag's universal stabilizer.

Chapter 3

Open Loop System

In this chapter we study the open loop CSTR system. For this purpose, first we try to find the equilibrium point of the system and then we consider the eigenvalues of the Jacobian. This will help us know more about the nature of the equilibrium point. This will bring us a better insight before applying Sontag's Theory.

3.1 EQUILIBRUIM POINT OF CSTR MODEL

In order to study the nature of the equilibrium point, we rewrite the system of nonlinear ODEs

$$\frac{dC_A}{dt} = \frac{F}{V_R}(C_{A0} - C_A) - C_A k_0 e^{\frac{-E}{RT_R}} \quad (3.1)$$

$$\frac{dT_R}{dt} = \frac{F}{V_R}(T_0 - T_R) - \frac{\lambda C_A k_0 e^{\frac{-E}{R T_R}}}{\rho c_p} - \frac{U A_J (T_R - T_J)}{V_R \rho c_p} \quad (3.2)$$

$$\frac{dT_J}{dt} = \frac{F_J}{V_J}\left(T_{C,in} - T_J\right) + \frac{U A_J (T_R - T_J)}{V_J \rho_J c_J} \quad (3.3)$$

Using the formulation [6]:

$$\dot{x}(t) = f\big(x(t)\big) + g\big(x(t)\big)\, u(t) \quad (3.4)$$

Where

$$x(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \\ x_3(t) \end{bmatrix} = \begin{bmatrix} C_A(t) \\ T_R(t) \\ T_J(t) \end{bmatrix} \quad (3.5)$$

$$f(x(t)) = \begin{bmatrix} \frac{F}{V_R}(C_{A0} - C_A) - C_A k_0 e^{\frac{-E}{RT_R}} \\ \frac{F}{V_R}(T_0 - T_R) - \frac{\lambda C_A k_0 e^{\frac{-E}{R T_R}}}{\rho c_p} - \frac{U A_J (T_R - T_J)}{V_R \rho c_p} \\ \frac{U A_J (T_R - T_J)}{V_J \rho_J c_p} \end{bmatrix} \quad (3.6)$$

$$g(x(t)) = \begin{bmatrix} 0 \\ 0 \\ \frac{(T_{C,in} - T_J)}{V_J} \end{bmatrix} \quad (3.7)$$

In order to find the equilibrium point we need to set the left hand side of Eq. (3.4) equal to zero, therefore

$$\dot{x}(t) = \begin{bmatrix} \frac{F}{V_R}(C_{A0} - C_A) - C_A\, k_0 e^{\frac{-E}{RT_R}} \\ \frac{F}{V_R}(T_0 - T_R) - \frac{\lambda\, C_A\, k_0 e^{\frac{-E}{R\,T_R}}}{\rho\, c_p} - \frac{U\, A_J\, (T_R - T_J)}{V_R\, \rho\, c_p} \\ \frac{U\, A_J\, (T_R - T_J)}{V_J\, \rho_J\, c_J} \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \frac{(T_{C,in} - T_J)}{V_J} \end{bmatrix} u(t) = 0 \quad (3.8)$$

Now, as it was mentioned before let the conversion χ of reactant A be

$$\chi = \frac{C_{A0} - C_A}{C_{A0}} \quad (3.9)$$

Let χ_{eq} be the chosen operating point reaction conversion. By (3.9) it follows that the operating point concentration of reactant in the reactor, $C_{A,eq}$ is given by

$$C_{A0}(1 - \chi_{eq}) \quad (3.10)$$

Now by substituting C_A by $C_{A,eq}$ in the first row of Eq. (3.8) we can find the equilibrium value for reactant temperature

$$T_{R,eq} = \frac{E}{R \ln\left(\frac{F\, \chi_{eq}}{k_0 V_R\, (1 - \chi_{eq})}\right)} \quad (3.11)$$

Similarly, by substituting equilibrium values for C_A and T_R in the second row of Eq. (3.8), we can find

$$T_{J,eq} = -\frac{F\, \rho\, c_p}{U\, A_J}\left(T_0 - T_{R,eq}\right) + \frac{\lambda\, C_{A,eq}\, k_0\, V_R\, e^{\frac{-E}{R\, T_{R,eq}}}}{U\, A_J} + T_{R,eq} \quad (3.12)$$

Consequently, by plugging all the equilibrium values in the third row of Eq. (3.8) we can find the equilibrium value for the rate of coolant flow by

$$F_{J,eq} = \frac{U\,A_J\,(T_{R,eq} - T_{J,eq})}{\rho_J\,c_J\,(T_{C,in} - T_{J,eq})} \quad (3.13)$$

In the next chapters, you will see that we consider F_J as the input of the open loop system, i.e. We manipulate cooling water flow rate to maintain the reaction conversion, the reactor temperature, and the jacket temperature at the chosen operating point. And while applying the Sontag's theory, the constructed nonlinear control input will be added to $F_{J,eq}$, and the sum will serve as the input of the closed loop system.

3.2 NATURE OF EQUILIBRUIM POINT

In this subchapter we are interested to study the nature of the equilibrium point in order to have a better intuition about the system's behavior at equilibrium point. If the equilibrium is asymptotically stable or just stable, we might not need to implant the stabilizing feedback. Obviously it's not the case, so we expect to observe that the system is unstable at its equilibrium. Following the classical way of studying the stability of dynamical systems, we will look for eigenvalues of the system's Jacobean. If there is positive real eigenvalues or imaginary ones with positive real part, it can rigidly prove the instability of the system.

The system of Eqs. (3.4) can be written as

$$\dot{x}(t) = f\big(x(t)\big) + g\big(x(t)\big)\,u(t) = h(x(t), t) \quad (3.14)$$

Where

$$h(x(t), t) = \begin{bmatrix} h_1(x(t), t) \\ h_2(x(t), t) \\ h_3(x(t), t) \end{bmatrix} \quad (3.15)$$

$$x(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \\ x_3(t) \end{bmatrix} = \begin{bmatrix} C_A(t) \\ T_R(t) \\ T_J(t) \end{bmatrix} \quad (3.16)$$

And the Jacobian of system is

$$J = \frac{\partial(h_1, h_2, h_3)}{\partial(x_1, x_2, x_3)} = \begin{bmatrix} \frac{\partial h_1}{\partial x_1} & \frac{\partial h_1}{\partial x_2} & \frac{\partial h_1}{\partial x_3} \\ \frac{\partial h_2}{\partial x_1} & \frac{\partial h_2}{\partial x_2} & \frac{\partial h_2}{\partial x_3} \\ \frac{\partial h_3}{\partial x_1} & \frac{\partial h_3}{\partial x_2} & \frac{\partial h_3}{\partial x_3} \end{bmatrix} \quad (3.16)$$

$$= \begin{bmatrix} -\frac{k_0}{e^{\frac{E}{RT_R}}}-\frac{F}{V_R} & -\frac{E\,k_0\,C_A}{R\,T_R{}^2\,e^{\frac{E}{RT_R}}} & 0 \\ -\frac{k_0\,\lambda}{\rho\,c_p\,e^{\frac{E}{RT_R}}} & -\frac{F}{V_R}-\frac{U\,A_J}{\rho\,c_p\,V_R}-\frac{E\,k_0\,\lambda\,C_A}{\rho\,c_p\,R\,T_R{}^2\,e^{\frac{E}{RT_R}}} & \frac{U\,A_J}{\rho\,c_p\,V_R} \\ 0 & \frac{U\,A_J}{\rho_J\,c_J\,V_J} & -\frac{29}{1250\,V_J}-\frac{U\,A_J}{\rho_J\,c_J\,V_J} \end{bmatrix} \quad (3.17)$$

Then by substituting x by equilibrium values, we have

$$J(x_{eq}) = \begin{bmatrix} -\frac{k_0}{e^{\frac{E}{RT_R},eq}}-\frac{F}{V_R} & -\frac{E\,k_0\,C_{A,eq}}{R\,T_R{}^2\,e^{\frac{E}{RT_R},eq}} & 0 \\ -\frac{k_0\,\lambda}{\rho\,c_p\,e^{\frac{E}{RT_R},eq}} & -\frac{F}{V_R}-\frac{U\,A_J}{\rho\,c_p\,V_R}-\frac{E\,k_0\,\lambda\,C_{A,eq}}{\rho\,c_p\,R\,T_{R,eq}{}^2\,e^{\frac{E}{RT_R},eq}} & \frac{U\,A_J}{\rho\,c_p\,V_R} \\ 0 & \frac{U\,A_J}{\rho_J\,c_J\,V_J} & -\frac{29}{1250\,V_J}-\frac{U\,A_J}{\rho_J\,c_J\,V_J} \end{bmatrix} \quad (3.18)$$

Where

$$x_{eq} = \begin{bmatrix} x_{1,eq} \\ x_{2,eq} \\ x_{3,eq} \end{bmatrix} = \begin{bmatrix} C_{A,eq} \\ T_{R,eq} \\ T_{J,eq} \end{bmatrix} \quad (3.19)$$

By calculating the eigenvalues of matrix (3.18) which has been done numerically in the next chapters you will see the system (3.14) has a negative real eigenvalues and a pair of complex conjugate eigenvalues with positive real part, which causes the steady state oscillation in the open loop system.

In the next chapter, we will review the Sontag's Universal Stabilizer theory. Then we will try to construct the control input as it's mentioned in Sontag's theory.

Chapter 4

Sontag's Theory on Nonlinear Stabilization

Several approaches to modern feedback design start with a control Lyapunov function for a system, and use the control Lyapunov function in order to construct a feedback stabilizer [7]. The Sontag’s theorem states that the existence of a smooth control-Lyapunov function implies smooth stabilizability [8]. In this chapter we state the feedback construction and Sontag’s theorem on nonlinear stabilization. Consequently, we will try to construct feedback design for CSTR model.

4.1 INTRODUCTION

This method concerns control systems of the type

$$\dot{x}(t) = f\big(x(t)\big) + g_1\big(x(t)\big)\, u_1(t) + g_2\big(x(t)\big)\, u_2(t) + \cdots + g_m\big(x(t)\big)\, u_m(t) \qquad (4.1)$$

With states $x(t) \in IR^n$ and controls $u(t) = \big(u_1(t), \ldots, u_m(t)\big) \in IR^m$ where f as well as the g_i's are smooth (i.e., infinitely differentiable,) vector fields and f(0) = 0. It is assumed that there is given a control Lyapunov function (henceforth just “clf’’) V for this system, that is, a smooth, proper, and positive definite function

$$V\colon IR^n \rightarrow IR$$

So that

$$\inf_{u \in IR^m}\{ L_f V(x) + u_1 L_{g1} V(x) + \cdots + u_m L_{gm} V(x)\} < 0 \qquad (4.2)$$

For each $x \neq 0$. In the other words, V is so that for each nonzero state x one can diminish its value by applying some open loop control. Recall that positive definite means that $V(0) = 0$ and $V(x) > 0$ for $x \neq 0$. And proper means that $V(x) \rightarrow \infty$ as $\|x\| \rightarrow \infty$ [8].

It is easy to show that the existence of such a clf implies that the system is asymptotically controllable (from any state one can asymptotically reach the origin); in the paper [9] it’s shown that the existence of a clf is in fact also necessary if there is asymptotic controllability, provided that one does not require smoothness (in which case Eq. (4.2) must be replaced by an equation involving Dini derivatives). More relevant to the topic of this paper, it was shown in [10] that if there is a clf, smooth as above, then there must be a feedback law

$$u = k(x), k(0) = 0 \quad (4.3)$$

This globally stabilizes the system and which is smooth on

$$\mathrm{IR}_0^n := \mathrm{IR}^n - 0$$

In general k may fail to be smooth everywhere, but under certain conditions, which we study later, k can be guaranteed to be at least continuous at the origin in addition to being smooth everywhere else [8].

4.2 FEEDBACK CONSTRUCTION

The construction is based on the following observation, which for introductory purposes we restrict to single-input (m = 1) systems only. Assume that V is a clf for the system

$$\dot{x}(t) = f\big(x(t)\big) + g\big(x(t)\big)u(t) \quad (4.4)$$

Denote

$$a(x) := \nabla V(x).f(x) \text{ and } b(x) := \nabla V(x).g(x) \quad (4.5)$$

The condition that V is clf is precisely the statement that

$$b(x) = 0 \ \Rightarrow a(x) < 0 \quad (4.6)$$

For all nonzero x. in other words, for each such x, the pair $\big(a(x), b(x)\big)$ is stabilizable.

When seen as a single-input, one-dimensional linear system. On the other hand, giving a feedback law $u = k(x)$ for the original system, with the property that the same V is a Lyapunov function for the obtained closed-loop system

$$\dot{x}(t) = f\big(x(t)\big) + g\big(x(t)\big)k(x) \quad (4.7)$$

Is equivalent to

$$\nabla V(x) \,.\, [f\big(x(t)\big) + g\big(x(t)\big)k(x)] < 0 \quad (4.8)$$

That is

$$a(x) + k(x)\, b(x) < 0 \quad (4.9)$$

For all nonzero x, In other words, k(x), seen as a 1×1 matrix, must be a constant linear feedback stabilizer for $\big(a(x), b(x)\big)$, for each fixed x. We now interpret $\big(a(x), b(x)\big)$, as a family of linear systems parameterized by x. This family depends smoothly on x. From the theory of families of systems or "systems over rings" we know that since each such linear system is stabilizable there exists indeed a smoothly dependent k as wanted. Moreover, this k can be chosen to be analytically or rationally dependent if the original family is, that is, if the original system and clf are [8]. The general theory is surveyed in [11], and the result in the smooth and analytic cases is due to [12], but in this very simple case (the family is one dimensional), the construction of k can be carried out directly without explicit recourse to the general result. Indeed, one can show directly that the following feedback law Works:

$$k := -\frac{a+\sqrt{a^2+b^2}}{b} \quad (4.10)$$

This results from the solution of an LQ problem, and is analytic, in fact algebraic, on a; b. (The apparent singularity due to division by b is removable, as discussed later.) Along trajectories of the corresponding closed-loop system, one has that

$$\frac{dV}{dt} = -\sqrt{a^2 + b^2} < 0 \quad (4.11)$$

As desired. This feedback law may fail to be continuous at zero, however. If one modifies it slightly to

$$k := -\frac{a+\sqrt{a^2+b^4}}{b} \quad (4.12)$$

Then under the natural hypotheses which are reviewed later this becomes continuous [8].

4.3 SONTAG'S THEORY

We start with some definitions for the system (4.1).

Definition let $k: IR^n \to IR^m$ be a mapping, smooth on IR_0^n and with $k(0) = 0$ this is a smooth feedback stabilizer for the system (4.1) provided that, with $k = (k_1, \dots, k_m)'$, the closed loop system

$$\dot{x}(t) = f\big(x(t)\big) + g_1\big(x(t)\big)\,k_1(t) + g_2\big(x(t)\big)\,k_2(t) + \cdots + g_m\big(x(t)\big)\,k_m(t) \quad (4.13)$$

is globally asymptotically stable.

By global asymptotic stability we mean the usual concept: attraction (solutions are defined for $t \geq 0$ and every initial state, and converge to 0) plus local asymptotic stability (initial states produce trajectories near the origin). The fact that k may fail to be even continuous at the origin causes no problems regarding uniqueness of solutions, as is easy to verify from the definition of asymptotic stability. A sufficient (as well as necessary) condition for a given k to be a smooth feedback stabilizer is that there exist a Lyapunov function for the closed-loop system, i.e. a smooth, proper, and positive definite function V so that

$$\nabla V(x) \, . \, [\, f(x(t)) + g_1(x(t))\, k_1(t) + g_2(x(t))\, k_2(t) + \cdots + g_m(x(t))\, k_m(t)\,] < 0 \quad (4.14)$$

For all nonzero x. Observe that such a Lyapunov function is automatically a clf for the open loop system (4.1). Note also that if k happens to be continuous at the origin then the following property holds too (with $u := k(x)$):

For each $\varepsilon > 0$ there is a $\delta > 0$ such that, if $x \neq 0$ satisfies $\|x\| < \delta$ then there is some u with $\|u\| < \varepsilon$ such that

$$\nabla V(x). f(x) + u_1 \nabla V(x) g_1(x) + \cdots + u_m \nabla V(x) g_m(x) < 0 \quad (4.15)$$

We shall call this the small control property for the clf V. The existence of a clf with this property is necessary if there is any smooth stabilizer continuous at zero; part of Artstein's theorem is the statement that this is also sufficient [7].

Theorem If there is a smooth clf V (respectively, the system as well as V are real analytic) then there is a smooth (respectively, real-analytic) feedback stabilizer k. If V satisfies the small control property, then k can be chosen to be also continuous at zero [7].

For the proof you might take a look on [8].

4.4 CSTR FEEDBACK DESIGN

In order to construct the CSTR feedback considering Sontag stabilizer we should study system's behavior locally. Therefore by a translation to equilibrium point we can construct the feedback in the neighborhood of equilibrium point. By recalling Eqs. (3.5) – (3.9) and (3.19), we define the new system's variable

$$y = x(t) - x_{eq} = \begin{bmatrix} y_1(t) \\ y_2(t) \\ y_3(t) \end{bmatrix} = \begin{bmatrix} C_A(t) - C_{A,eq} \\ T_R(t) - T_{R,eq} \\ T_J(t) - T_{J,eq} \end{bmatrix} \quad (4.16)$$

And for clf we suggest quadratic form:

$$\mathrm{W}: \mathrm{IR}^3 \to \mathrm{IR} \quad \text{and} \quad \mathrm{W} = \mathrm{y}' \mathrm{P}\, \mathrm{y} \qquad (4.17)$$

Where P is symmetric positive definite. Then by rewriting the f and g in terms of y

$$\mathrm{F}\big(\mathrm{y}(\mathrm{t})\big) =$$

$$\begin{bmatrix} \frac{\mathrm{F}}{\mathrm{V_R}}(\mathrm{C_{A0}} - (\mathrm{C_A} - \mathrm{C_{A,eq}})) - (\mathrm{C_A} - \mathrm{C_{A,eq}})\, \mathrm{k_0} e^{\frac{-\mathrm{E}}{\mathrm{R}(\mathrm{T_R} - \mathrm{T_{R,eq}})}} \\ \frac{\mathrm{F}}{\mathrm{V_R}}\Big(\mathrm{T_0} - (\mathrm{T_R} - \mathrm{T_{R,eq}})\Big) - \frac{\lambda\, (\mathrm{C_A} - \mathrm{C_{A,eq}})\, \mathrm{k_0} e^{\frac{-\mathrm{E}}{\mathrm{R}(\mathrm{T_R} - \mathrm{T_{R,eq}})}}}{\rho\, \mathrm{c_p}} - \frac{\mathrm{U\, A_J}\, ((\mathrm{T_R} - \mathrm{T_{R,eq}}) - (\mathrm{T_J}(\mathrm{t}) - \mathrm{T_{J,eq}}))}{\mathrm{V_R}\, \rho\, \mathrm{c_p}} \\ \frac{\mathrm{U\, A_J}\, ((\mathrm{T_R} - \mathrm{T_{R,eq}}) - (\mathrm{T_J}(\mathrm{t}) - \mathrm{T_{J,eq}}))}{\mathrm{V_J}\, \rho_\mathrm{J}\, \mathrm{c_J}} \end{bmatrix} \qquad (4.18)$$

$$\mathrm{G}(\mathrm{y}(\mathrm{t})) = \begin{bmatrix} 0 \\ 0 \\ \frac{(\mathrm{T_{C,in}} - (\mathrm{T_J}(\mathrm{t}) - \mathrm{T_{J,eq}}))}{\mathrm{V_J}} \end{bmatrix} \qquad (4.19)$$

Therefore by recalling Eq. (4.5)

$$\mathrm{a}: \mathrm{IR}^3 \to \mathrm{IR} \quad \text{and} \quad \mathrm{a} = \nabla \mathrm{W}.\, \mathrm{F}(\mathrm{y}) \qquad (4.20)$$

$$\mathrm{b}: \mathrm{IR}^3 \to \mathrm{IR} \quad \text{and} \quad \mathrm{b} = \nabla \mathrm{W}.\, \mathrm{G}(\mathrm{y}) \qquad (4.21)$$

And since P is symmetric positive definite, $\nabla \mathrm{W} = 2\, \mathrm{y}' \mathrm{P}'$ therefore

$$\mathrm{a} = 2\, \mathrm{y}' \mathrm{P}' \mathrm{F}(\mathrm{y}) \quad \text{and} \quad \mathrm{b} = 2\, \mathrm{y}' \mathrm{P}' \mathrm{G}(\mathrm{y}) \qquad (4.22)$$

Now by plugging in these scalar values of a and b into Eq. (4.12), we can find the stabilizing feedback as

$$\mathrm{k} := -\frac{[2\, \mathrm{y}' \mathrm{P}' \mathrm{F}(\mathrm{y})] + \sqrt{[2\, \mathrm{y}' \mathrm{P}' \mathrm{F}(\mathrm{y})]^2 + [2\, \mathrm{y}' \mathrm{P}' \mathrm{G}(\mathrm{y})]^4}}{2\, \mathrm{y}' \mathrm{P}' \mathrm{G}(\mathrm{y})} \qquad (4.23.1)$$

In the next chapters, you will see that when we are studying the closed loop system, $(\mathrm{F_j} + \mathrm{k})$ will be considered as the input of the system. So the rate of coolant flow will be adjusted according to Sontag theorem. As you can see the (4.12) becomes discontinuous when b goes to zero. When this happens, solving the system of ODEs is impossible. In order to solve this problem, we slightly modify the feedback input [13]. Therefore we choose the feedback input as

$$k(y) = \begin{cases} -\frac{a(y)+\sqrt{a(y)^2+b(y)^4}}{b(y)} & \text{if } |b| > r \\ -\frac{\left(a(y)+\sqrt{a(y)^2+b(y)^4}\right)\, .\, b(y)}{r^2} & \text{if } |b| \le r \end{cases} \qquad (4.23.2)$$

Where r is chosen very small according to [13].

4.5 REVISITING THE CLF CONSIDERING FEEDBACK DESIGN

In this subchapter we construct the stabilizer pair $\left(a(x), b(x)\right)$ using a symmetric positive definite matrix P. Consequently, we will consider condition (4.6) to make sure V is indeed clf for the CSTR system.

Consider the fact that for many choices of positive definite matrices for P, the pair $\left(a(x), b(x)\right)$ is not satisfying condition (4.6). Therefore, we started by taking identity matrix and tuning it in order to preserve positive definiteness and satisfy (4.6). The resulting matrix P is:

$$P = \begin{bmatrix} 501 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 1 \end{bmatrix} \quad \lambda_1 = 0.3818 \quad \lambda_2 = 2.6142 \quad \lambda_3 = 501.0040$$

Now by recalling Eqs. (4.22) and (4.16) we construct the pair $\left(a(x), b(x)\right)$ using this matrix P

$$a(y) = \left[\left(\frac{\left(2UA_J(y_2-y_3)(y_1+y_2+y_3)\right)}{V_J\,\rho_J\,c_J}\right) - \left(\frac{\lambda k_0 y_1}{\rho\, c_p\, e^{\frac{E}{Ry_2}}} - \frac{F(T_0-y_2)}{V_R} + \frac{UA_J(y_2-y_3)}{V_R\,\rho\,c_p}\right)(2y_1 + 4y_2 + 2y_3) - \left(\frac{k_0 y_1}{e^{\frac{E}{Ry_2}}} - \frac{F(C_{A0}-y_1)}{V_R}\right)(1002y_1 + 2y_2 + 2y_3)\right] \qquad (4.24)$$

$$b(y) = \left[\frac{2\,(T_{C,in}-y_3)\,(y_1+y_2+y_3)}{V_J}\right] \qquad (4.25)$$

By considering condition (4.6) in order make sure that the suggested quadratic form is indeed clf of the system, when $b(y)$ is equal to zero, $a(y)$ should be negative. Therefore we need to evaluate Eq. (4.24) at the nonzero roots of (4.25).

$$b(y) = 0 \Rightarrow y_{01} = (0,0,0) \text{ or } y_{02} = \left(y_1, y_2, T_{C,in}\right) \text{ or } y_{03} = (-(y_1 + y_3), y_2, y_3) \qquad (4.26)$$

Now, for the nonzero roots of $\mathrm{b(y)}$ (i.e. $\mathrm{y_{02}}$ and $\mathrm{y_{03}}$) we plotted $\mathrm{a(y)}$ using Matlab. Considering Figures (4.1) and (4.2) we can see that for the nonzero roots of $\mathrm{b(y)}$, $\mathrm{a(y)}$ is negative, therefore according to (4.6) the quadratic form is clf and the pair $(\mathrm{a(y)}, \mathrm{b(y)})$ is stabilizer.

In the next chapter we will give a brief explanation about the implemented program in Matlab regarding the model and controller. Then it follows by simulation results for the open loop and closed loop system.

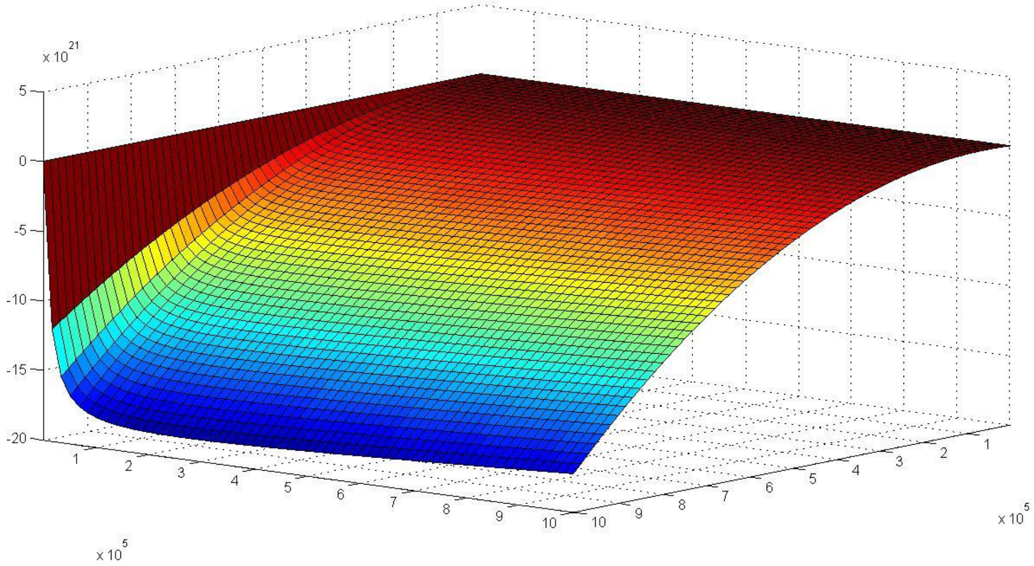


Figure 4.1: $\mathbf{a(y)}$ evaluated at the $\mathbf{y_{02}} = \left(\mathbf{y_1}, \mathbf{y_2}, \mathbf{T_{C,in}}\right)$

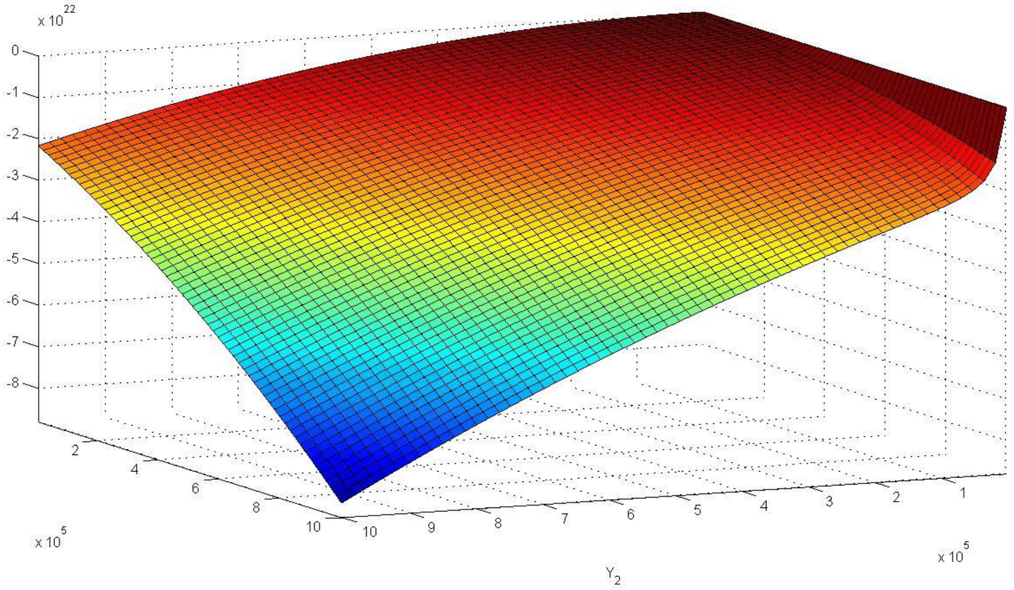


Figure 4.2: $\mathbf{a(y)}$ evaluated at the $\mathbf{y_{03}} = (-(\mathbf{y_1} + \mathbf{y_3}), \mathbf{y_2}, \mathbf{y_3})$

Chapter 5

Implementation in Matlab

In this chapter the implemented program in Matlab will be studied. We have implemented jacket cooled CSTR in order to study open loop system. Consequently, by observing the fact that the equilibrium is unstable we will apply Sontag stabilizer as the feedback for closed loop system. In this case, when the stabilizing input is discontinuous, we modified the feedback using the method which is discussed in [13]. In the next chapter the simulation result will be shown.

5.1 PARAMETERS

System's parameter values which have been considered in simulations are:

C_{A0} = 8.01 ($\frac{\mathrm{kmol}}{\mathrm{m}^3}$) ; k_0= 20.75$\times 10^{-6}$ (s^{-1}) ; E = 69.71$\times 10^{6}$ ($\frac{\mathrm{J}}{\mathrm{kmol}}$)

R = 8314 (J kmol^{-1} K^{-1}) ; $\lambda = -69.71 \times 10^{6}$ ($\frac{\mathrm{J}}{\mathrm{kmol}}$) ; ρ = 801 ($\frac{\mathrm{kg}}{\mathrm{m}^3}$)

c_p = 3137 (J kg^{-1} K^{-1}) ; $\rho_J = 1000$ ($\frac{\mathrm{kg}}{\mathrm{m}^3}$) ; c_J= 4183 (J kg^{-1} K^{-1})

$T_{C,in}$= 294 (K) ; F = 4.377 $\times 10^{-3}$ ($\frac{\mathrm{m}^3}{\mathrm{s}}$) ; V_R = 102 (m^3)

U = 851 (W K^{-1} m^{-2}) ; A_J=102 (m^2) ; V_J=10.1 (m^2); T_0 = 294 (K)

The set of parameters has been taken from [6].

5.2 EQUILIBRIUM POINT, EIGENVALUES AND JACOBIAN

5.2.1 Equilibrium Point

In order to make sure the equilibrium values calculated in [6] are precise, we tried to compute them again by using above parameters. Therefore, by considering Eqs. (3.10) to (3.13) we wrote a very simple code to find the values in Matlab. The program can be found in the section A.1.

5.2.2 Eigenvalues and System's Jacobian

Prior to studying open loop and closed loop system, it seemed crucial to have an idea about the nature of equilibrium. Regarding the theoretic argument in the section 3.2, we implemented a very simple algorithm (Section A.2) to find the system's Jacobian (Eq. 3.17). Therefore by replacing the variables by equilibrium values (Eq. 3.18) and finding the eigenvalues of this matrix, we made sure that the equilibrium is unstable.

5.3 OPEN LOOP SYSTEM

The program implemented to study open loop behavior includes two separated codes, in the first one (Section A.3.1) we wrote a function which generates the CSTR nonlinear dynamics (Eqs. 3.1 to 3.3). It should be taken into consideration that since the coolant flow rate (F_J) appears in the third ODE, therefore you can modify its initial value in the section A.3.1. The second part of program (Section A.3.2) is to solve the system of ODEs. For this purpose we used the ode45 solver which is already developed in Matlab library. Since, the system doesn't reach the saturation state, so it's not necessary to change time step for the solver. You can modify the integration time span and the variable's initial values in this part of the program.

5.4 CLOSED LOOP SYSTEM

Similar to open loop system, the program (Section A.4) for applying Sontag's stabilizer to CSTR model consists of two parts. The first part is similar to section A.3.1; moreover the feedback construction is embedded in the code. By considering the section 4.3 the feedback is built by suggesting a proper positive definite matrix. It may happen that $b(y)$ becomes approximately zero; therefore the feedback formula (Eq. 4.12) doesn't make sense anymore. In order to solve this problem we used the Method which is discussed in [13]. The method is shortly explained at the end of section 4.3. In the second part of the program (Section A.4.2), we used ode15tb for solving the system of ODEs.

5.5 CONSIDERING CLF CONDITION IN TERMS OF a(y) AND b(y)

In order to conclude that if the suggested Lyapunov is indeed clf we can check if the condition (4.6) is satisfied. Therefore, after finding the roots of $b(y)$, we can evaluate the sign of $a(y)$ by plotting it. In the program (Section A.5) it is also possible to see the symbolic formula of $a(y)$ and $b(y)$.

In the next chapter we will review the simulation results of the implemented programs.

Chapter 6

Simulation Results

In this chapter we discuss the simulation results regarding Jacket cooled CSTR model. It starts by showing the fact that some of the eigenvalues of the system's Jacobian are positive, therefore system is unstable. Then it follows by studying open loop and closed loop behavior of the system. The main point of this simulation is to gain smooth convergence of closed loop behavior to equilibrium values.

6.1 EQUILIBRIUM VALUES

Using the program which can be found in the section A1, by using the parameters from section 5.1 the equilibrium point is calculated:

$$\mathrm{x_{eq}} = \begin{bmatrix} \mathrm{x_{1,eq}} \\ \mathrm{x_{2,eq}} \\ \mathrm{x_{3,eq}} \end{bmatrix} = \begin{bmatrix} \mathrm{C_{A,eq}} \\ \mathrm{T_{R,eq}} \\ \mathrm{T_{J,eq}} \end{bmatrix} = \begin{bmatrix} 1.6020 \\ 328.5763 \\ 310.2527 \end{bmatrix} \quad (6.1)$$

By considering these values the equilibrium coolant flow rate is:

$$\mathrm{F_{J,eq}} = 0.0232 \quad (6.2)$$

These values are considered as equilibrium values it the other simulations.

6.2 EIGENVALUES OF JACOBIAN

By running the program which is attached in the section A.2, the eigenvalues of system's Jacobian are:

$$\lambda_1 = 0.0001 - 0.0001i \quad , \quad \lambda_2 = 0.0001 + 0.0001i \quad , \quad \lambda_3 = -0.0045 \quad (6.3)$$

As you can see there is a pair of complex conjugate eigenvalues with positive real part, therefore we expect an oscillating open loop behavior.

6.3 OPEN LOOP BEHAVIOR

As it is shown in the previous section, CSTR model has a pair of complex eigenvalues with positive real part, therefore it's unstable. In the coming simulation, coolant flow rate F_J is considered as input. Reactant concentration, reactant and jacket temperatures are the system's state variables, which are also the outputs. We have considered three different test cases for the open loop system.

- Case 1: Initial values and input equal to equilibrium.
- Case 2: Initial values equal to equilibrium values with an input far from equilibrium.
- Case 3: Initial values far from the equilibrium and the input equal to equilibrium.

The result is respectively shown in Fig. 6.1 to Fig. 6.3.

6.4 CLOSED LOOP BEHAVIOR

Using the theoretic arguments which discussed in the chapter 4, we implemented the Sontag's stabilizing feedback for jacket cooled CSTR model. As it is stated at the end of section 4.3, when the stabilizing feedback goes to zero we used the alternate feedback design according to [13]. It should be taken into consideration this modification results in a bounded Lipschitz continues control feedback. In the figures 6.4 to 6.6 you can see the simulation results of the test cases for the stabilized system, except in this case the input is constructed using the construction discussed in section 4.3. The positive definite matrix P is chosen experimentally, i.e. by trying many PD matrices and preserving symmetry and positive definiteness.

$$P = \begin{bmatrix} 10.00001 & 0.0000005 & 0.00000001 \\ 0.0000005 & 0.0000101 & 0.00000001 \\ 0.00000001 & 0.00000001 & 0.0000101 \end{bmatrix} \quad (6.4)$$

$$\lambda_1 = 0.00001 \quad \lambda_2 = 0.00001 \quad \lambda_3 = 10.00001$$

Therefore P is positive definite and it fits the theorem.

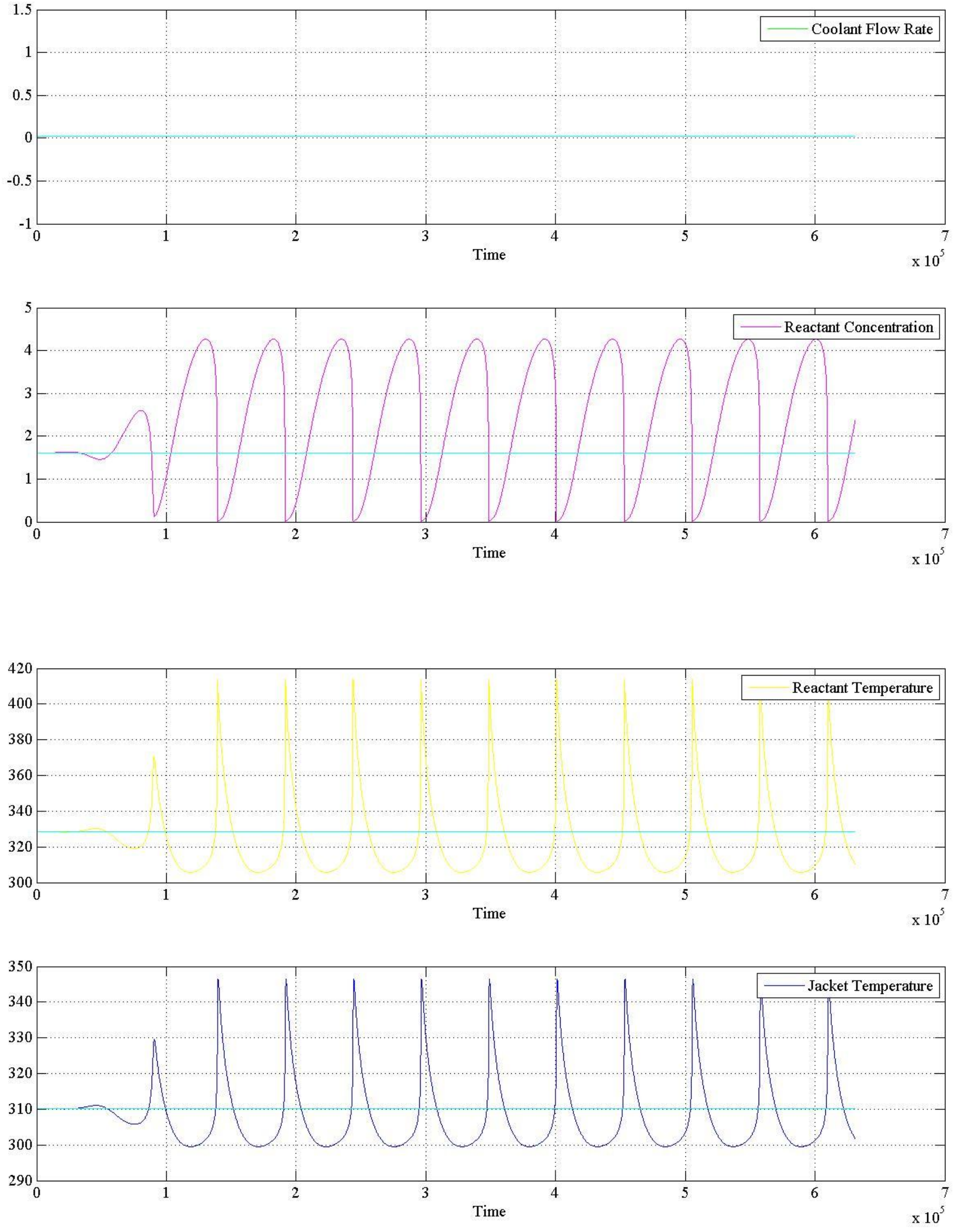


Figure 6.1: Open Loop Behavior, Case 1. Initial Values and Input Are Equal to Equilibrium Values.

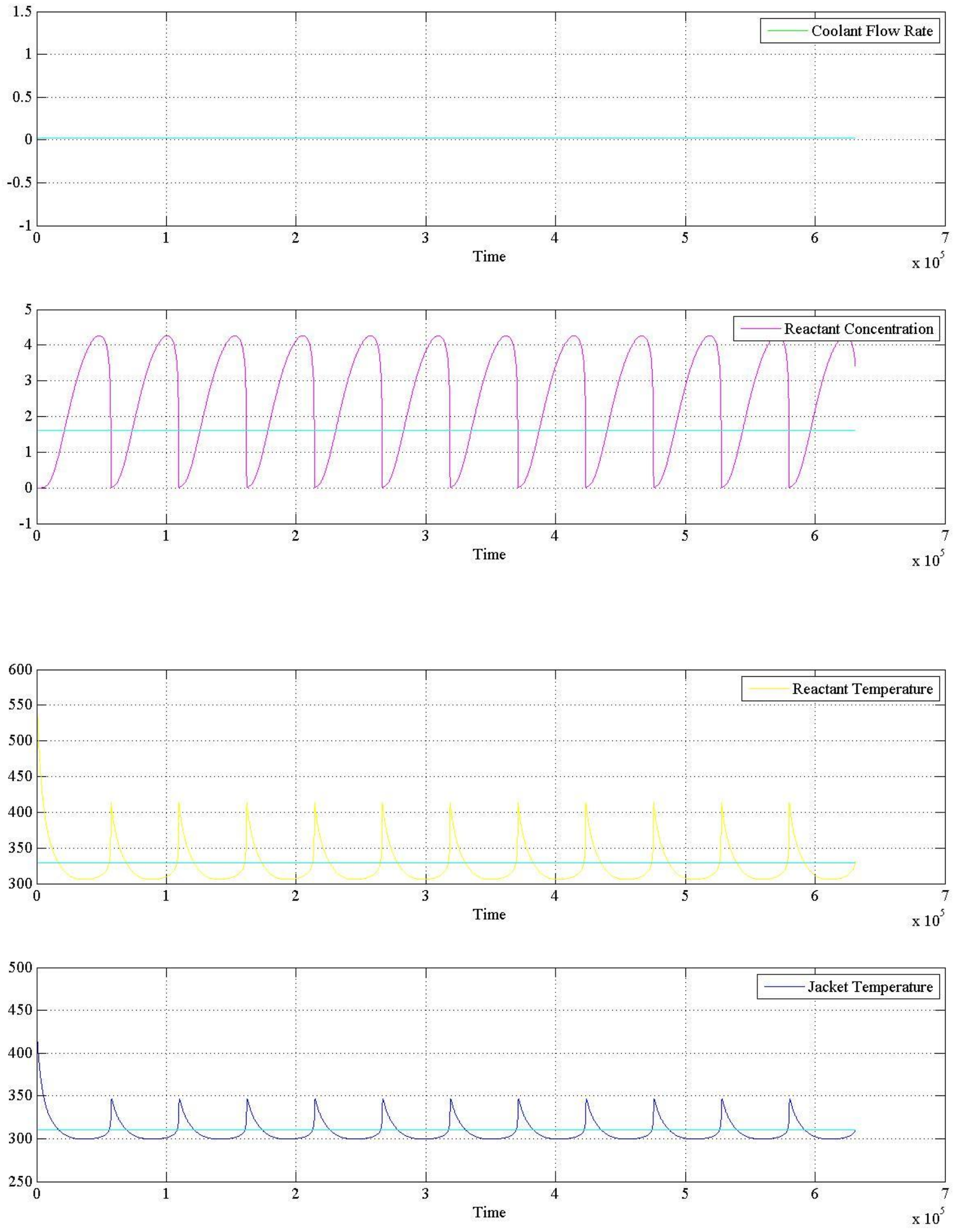


Figure 6.2: Open Loop Behavior, Case 2. Initial Values Are Far From Equilibrium Values and the Input Is Equal to Equilibrium.

$$\mathbf{(x_1(0) = 1.5\, x_{1,eq},\ x_2(0) = 1.5\, x_{2,eq},\ x_3(0) = 1.5\, x_{3,eq},\ F_J = F_{J,eq}).}$$

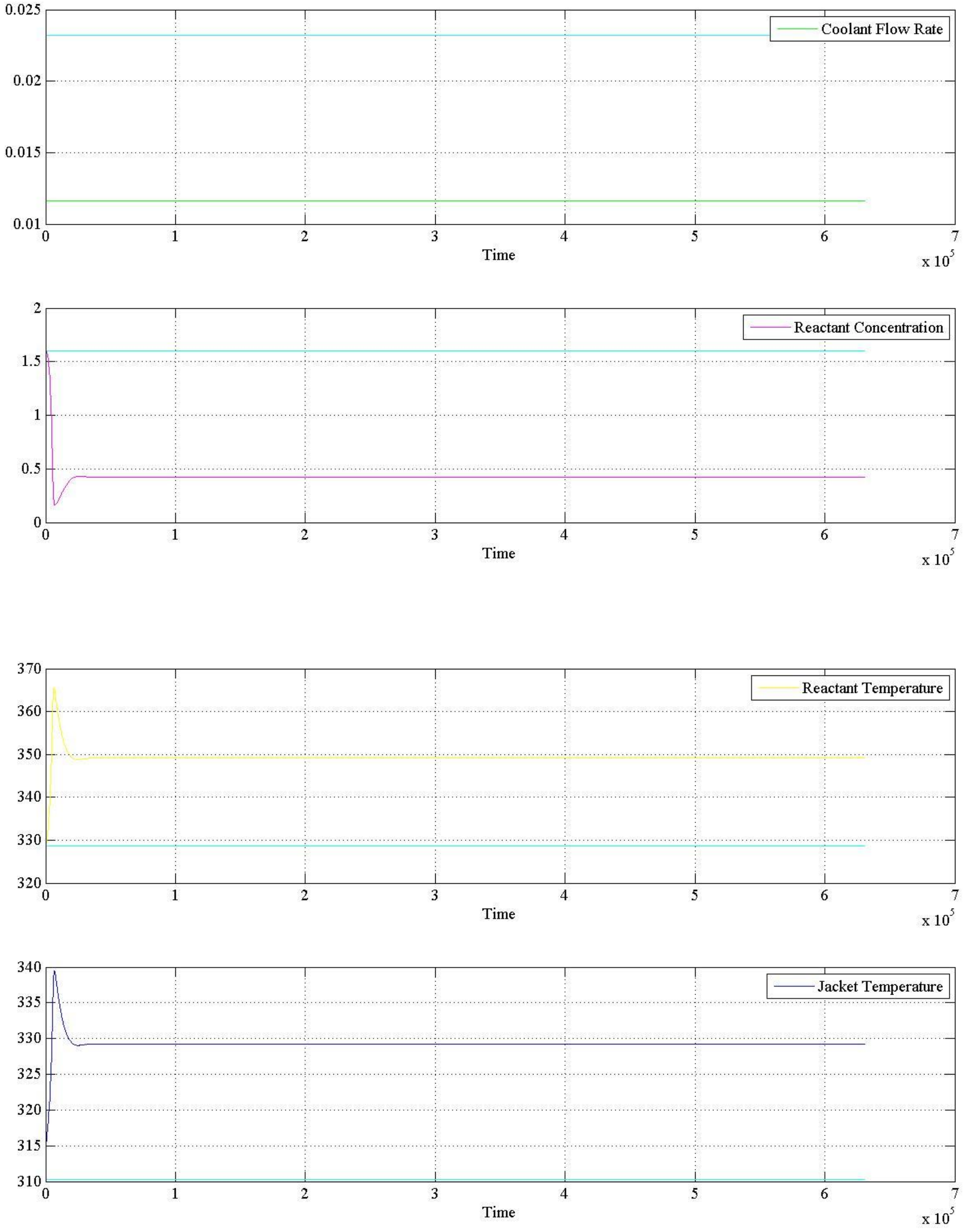


Figure 6.3: Open Loop Behavior, Case 3. Initial Values Are Equal to Equilibrium Values and the Input Is Far From Equilibrium.

$$\mathbf{(x_1(0) = x_{1,eq},\ x_2(0) = x_{2,eq},\ x_3(0) = x_{3,eq},\ F_J = 0.5\ F_{J,eq})}$$

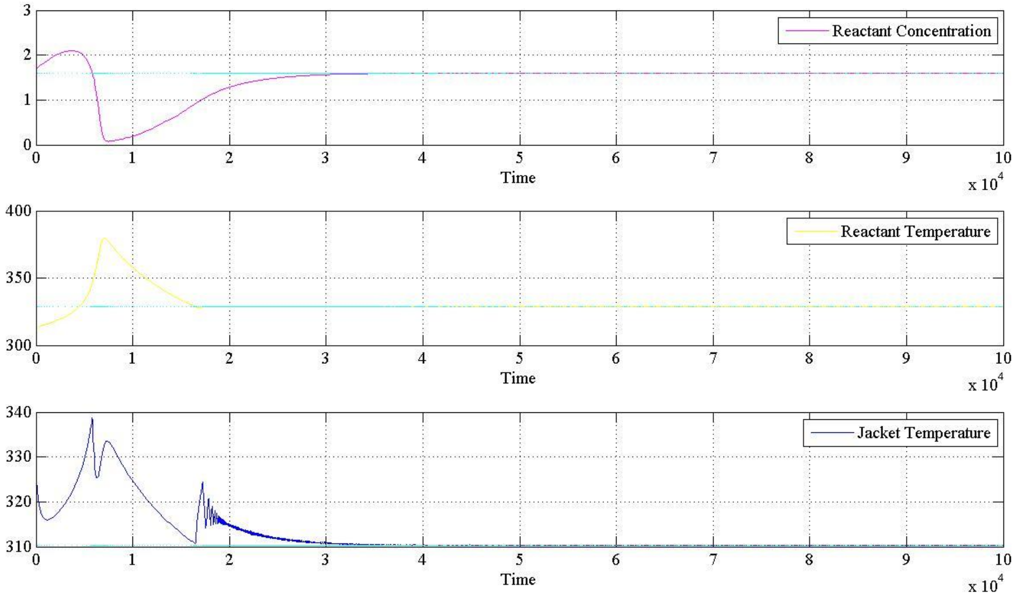


Figure 6.4: Closed Loop Behavior, Case 1.

$(\mathbf{x_1(0) = 1.05\, x_{1,eq}},\ \mathbf{x_2(0) = 0.95\, x_{2,eq}},\ \mathbf{x_3(0) = 1.05\, x_{3,eq}})$

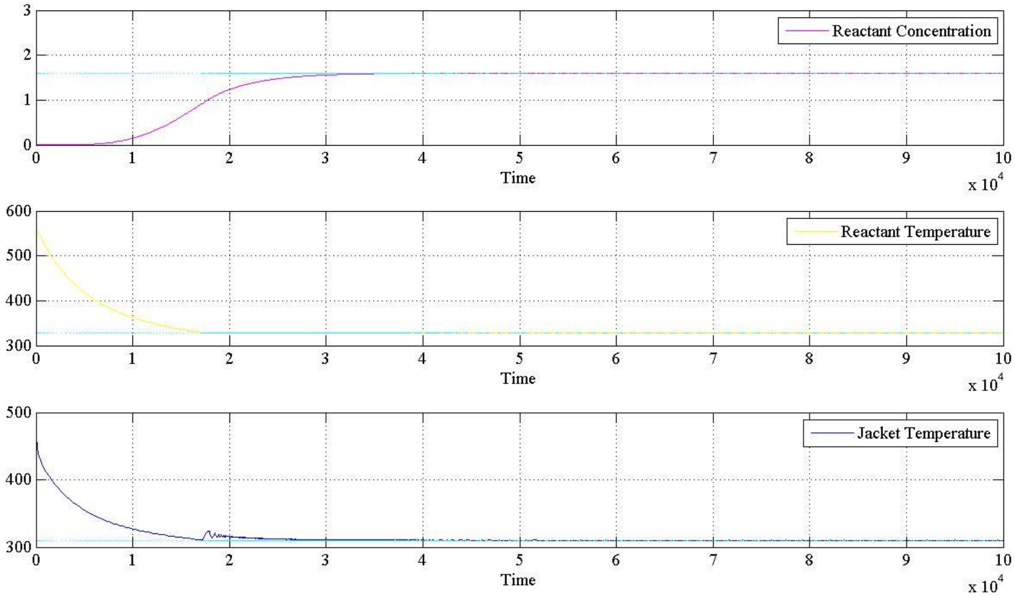


Figure 6.5: Closed Loop Behavior, Case 2.

$(\mathbf{x_1(0) = 1.50\, x_{1,eq}},\ \mathbf{x_2(0) = 1.50\, x_{2,eq}},\ \mathbf{x_3(0) = 1.50\, x_{3,eq}})$

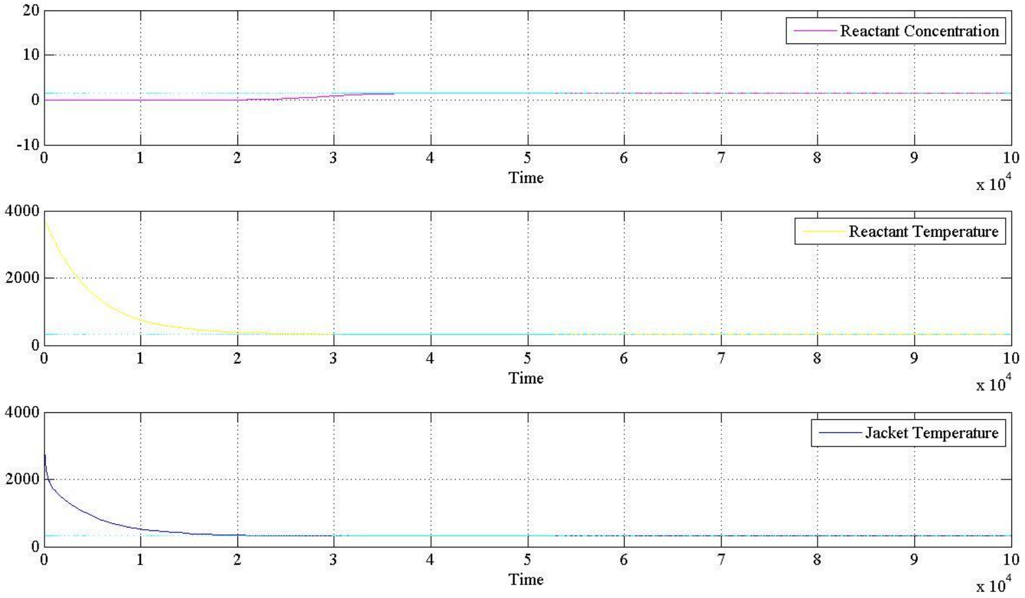


Figure 6.6: Closed Loop Behavior, Case 3.

$(\mathbf{x_1(0) = 10\ x_{1,eq},\ \ x_2(0) = 10\ x_{2,eq},\ \ x_3(0) = 10\ x_{3,eq}})$

The methodology that we have adopted in order to stabilize the CSTR model is rather new. Therefore applying Sontag’s stabilizer to CSTR model requires more theoretical consideration to gain a nicer feedback. We call it nicer to point out the fact that the feedback constructed by Sontag’s theorem may have some properties such as complete and locally Lipschitz continuity. According to [13] if the designed controller parameters $a(y)$ and $b(y)$ for $\alpha_1, \alpha_2, \alpha_3$ of class K_∞ and positive real r and p, satisfy below hypotheses:

$$\alpha_1(|y|) \le V(y) \le \alpha_2(|y|)$$

$$b(y) = 0 \; \Rightarrow a(y) \le 0$$

$$a^2(y) + |b(y)|^2 \ge {\alpha_3}^2(|y|)$$

$$\mathrm{Sup}_{\{y \,\epsilon\, IR^n, 0<|b(y)|\le r\}} \frac{a(y)}{|b(y)|} \le p$$

Then according to theorem 9 in [13], the feedback input

$$k(y) = \begin{cases} -\dfrac{a(y) + \sqrt{a(y)^2 + b(y)^4}}{b(y)} & \text{if } |b| > r \\ -\dfrac{\left(a(y) + \sqrt{a(y)^2 + b(y)^4}\right) \,.\, b(y)}{r^2} & \text{if } |b| \le r \end{cases}$$

Is completely and locally Lipschitz continuous, in addition by considering the stabilizing input as $u(t) = k(y) - qb^T(y)$ then the solution exists for all $t \ge 0$, where q is the tuning parameter, the closed loop system with a bounded additive disturbance $d(t)$ can approach any arbitrary neighborhood of the origin by increasing the tuning parameter.

Moreover, CSTR feedback design can be studied as a discrete problem. In the other word, the system’s output can be discretized by sampling. Then the controller will be designed in discrete form. Consequently, the continuous stabilizing input can be generated by using zero order hold (ZOH) signal reconstruction block.

Apendices

It might be questionable that why for every single section the parameters and equilibrium values are attached. The reason was to make it easier for the readers to check the results of every section just by copying the code to Matlab.

A.1 PARAMETERS, INTERGRATION TIME SPAN AND INITIAL VALUES

```
%---Model Parameters--------------------------------------------
CA_0 = 8.01;Lambda = - 69.71*10^6;
E = 69.71*10^6;
Cp = 3137;Cj = 4183;F = 4.377*10^-3;U = 851;
Vj = 10.1;K_0 = 20.75*10^6;R = 8314;
Ro = 801;Roj = 1000;Tc_in = 294;
Vr = 102;Aj = 101;T_0 = 294;
%---Calculating the Equilibrium Values--------------------------
% Reaction Conversion
Re_con = 0.80;
% Reactant Concentration
CA_eq=CA_0*(1-Re_con)
% Reactant Temperature
Tr_eq=-E/(R*log((F*Re_con)/(K_0*Vr*(1-Re_con))))
% Jacket Temperature
Tj_eq=-((F*Cp*Ro)/(U*Aj))*(T_0-Tr_eq)+(Lambda*CA_eq*K_0*Vr*exp(-
E/(R*Tr_eq)))/(U*Aj)+Tr_eq
% Coolant Flow Rate
Fj_eq=-((U*Aj*(Tr_eq-Tj_eq))/(Roj*Cj*(Tc_in-Tj_eq)))
%---Initial Values Deviation w.r.t. Equilibrium Values----------
CA_percentage=1;
Tr_percentage=1;
Tj_percentage=1;
X_eq=[CA_eq;Tr_eq;Tj_eq];
X0 =
[CA_percentage*CA_eq;Tr_percentage*Tr_eq;Tj_percentage*Tj_eq];
%---Coolant Flow Deviation w.r.t Equilibrium Values-------------
Flow_percentage=1;
Fj=Flow_percentage*Fj_eq;
%----Integration Time Span--------------------------------------
time_order=1;
time=10^time_order;
```

A.2 EQUILIBRIUM POINT, EIGENVALUES AND JACOBIAN

```
%---Parameters Values and Variables Definition------------------
syms x y z
CA_0 = 8.01; Lambda = - 69.71*10^6;
E = 69.71*10^6; Cp = 3137;
Cj = 4183; F = 4.377*10^-3;
U = 851; Vj = 10.1;
K_0 = 20.75*10^6; R = 8314;
Ro = 801; Roj = 1000;
Tc_in = 294; Vr = 102;
Aj = 101; T_0 = 294;
%---Equilibrium Values------------------------------------------
CA_eq = 1.6020; Tr_eq = 328.5763;
Tj_eq = 310.2527; Fj_eq = 0.0232;
%---Initial Values Deviation w.r.t. Equilibrium Values----------
CA_percentage=1;
Tr_percentage=1;
Tj_percentage=1;
X_eq=[CA_eq;Tr_eq;Tj_eq];
X0 =
[CA_percentage*CA_eq;Tr_percentage*Tr_eq;Tj_percentage*Tj_eq];
%---Coolant Flow Deviation w.r.t Equilibrium Values-------------
Flow_percentage=1;
Fj=Flow_percentage*Fj_eq;
%----Integration Time Span--------------------------------------
time_order=1;
time=10^time_order;
%---Jacobian and Eigenvalues------------------------------------
g=[(F/Vr)*(CA_0-x)-x*K_0*exp(-E/(R*y));
   (F/Vr)*(T_0-y)-(Lambda*x*K_0*exp(-E/(R*y)))/(Ro*Cp)-(U*Aj*(y-
z))/(Vr*Ro*Cp);
   (Fj/Vj)*(Tc_in-z) + (U*Aj*(y-z))/(Vj*Roj*Cj)];
Jacobian=jacobian (g,[x,y,z])
p=eig(jacobian (g,[x,y,z]))
eigenvalues=subs(p,{x,y,z},{CA_eq,Tr_eq,Tj_eq})
```

A.3 OPEN LOOP SYSTEM

A.3.1 System of ODEs

```
function [dX,X] = CSTR2(~,X)

CA_0 = 8.01; Lambda = - 69.71*10^6;
E = 69.71*10^6; Cp = 3137;
Cj = 4183; F = 4.377*10^-3;
U = 851; Vj = 10.1;
K_0 = 20.75*10^6; R = 8314;
Ro = 801; Roj = 1000;
Tc_in = 294; Vr = 102;
Aj = 101; T_0 = 294;

Flow_percentage=1;
Fj_eq = 0.0232;
Fj=Flow_percentage*Fj_eq;
%---Generating the System of ODEs-------------------------------
dX = zeros(3,1);
dX(1) = (F/Vr)*(CA_0-X(1))-X(1)*K_0*exp(-E/(R*X(2)));
dX(2) = (F/Vr)*(T_0-X(2))-(Lambda*X(1)*K_0*exp(-
E/(R*X(2))))/(Ro*Cp)-(U*Aj*(X(2)-X(3)))/(Vr*Ro*Cp);
dX(3) = ((Fj)/Vj)*(Tc_in-X(3)) + (U*Aj*(X(2)-X(3)))/(Vj*Roj*Cj);

end
```

A.3.2 Solving System of ODEs

```
clc
close all
CA_percentage=1;
Tr_percentage=1;
Tj_percentage=1;
time_order=5.8;

CA_eq = 1.6020; Tr_eq = 328.5763;Tj_eq = 310.2527;
X0 =
[CA_percentage*CA_eq;Tr_percentage*Tr_eq;Tj_percentage*Tj_eq];
X_eq=[CA_eq;Tr_eq;Tj_eq];
time=10^time_order;

options = odeset('RelTol',1e-4,'AbsTol',[1e-4 1e-4 1e-5])
[T,X] = ode45(@CSTR2,[0 time],X0,options)
```

```
whitebg('w')
plot(T,X(:,1),'--',T,X(:,2),'--',T,X(:,3),'--')
legend('Reactanc Concentration','Reactant Temprature','Jacket
Temprature')
Grid on

figure
plot(T,X(:,1),'r',T,CA_eq,'b','LineWidth',1.2)
xlabel('Time')
legend('Reactant Concentration','Equilibrium Value')
grid on

figure
plot(T,X(:,2),'r',T,Tr_eq,'b','LineWidth',1.2)
xlabel('Time')
legend('Reactant Temperature','Equilibrium Value')
grid on

figure
plot(T,X(:,3),'r',T,Tj_eq,'b','LineWidth',1.2)
xlabel('Time')
legend('Jacket Temperature','Equilibrium Value')
grid on
```

A.4 CLOSED LOOP SYSTEM

A.4.1 Constructing the Feedback

```
function [dX,X] = CSTR2_Sontag(~,X)

CA_0 = 8.01; Lambda = - 69.71*10^6; E = 69.71*10^6;
Cp = 3137; Cj = 4183; F = 4.377*10^-3; U = 851;
Vj = 10.1; K_0 = 20.75*10^6; R = 8314;
Ro = 801; Roj = 1000; Tc_in = 294;
Vr = 102; Aj = 101; T_0 = 294;

CA_eq = 1.6020; Tr_eq = 328.5763;Tj_eq = 310.2527;
X_eq=[CA_eq;Tr_eq;Tj_eq];

P=10*10^-
6*(eye(3,3)+[1000000,0.05,0.001;0.05,0.01,0.001;0.001,0.001,0.01
]);
P_Eigenvalues=eig(P)

Y=[(X(1)-X_eq(1));(X(2)-X_eq(2));(X(3)-X_eq(3))];
```

```
%---Feedback Construction---------------------------------------

FF=[((F/Vr)*(CA_0-(X(1)-X_eq(1))))-((X(1)-X_eq(1))*K_0*exp(-
E/(R*(X(2)-X_eq(2)))));
   ((F/Vr)*(T_0-(X(2)-X_eq(2))))-((Lambda*(X(1)-
X_eq(1))*K_0*exp(-E/(R*(X(2)-X_eq(2)))))/(Ro*Cp))-((U*Aj*((X(2)-
X_eq(2))-(X(3)-X_eq(3))))/(Vr*Ro*Cp));
   (U*Aj*((X(2)-X_eq(2))-(X(3)-X_eq(3))))/(Vj*Roj*Cj)];

GG=[0;0;(1/Vj)*(Tc_in-(X(3)-X_eq(3)))];

a=FF'*2*P*Y;
b=GG'*2*P*Y;

%---Sontag’s Stabilizer Combined with Method of SCL-------------
r_SCL=10^(-5);

if abs(b)<=r_SCL,
    v=-((a+((a^2+b^4)^0.5)))*b/r_SCL^2;
else
v = -(a+((a^2+b^4)^0.5))/b;
end;

Flow_percentage=1;
Fj_eq =0.0232;
Fj=Flow_percentage*Fj_eq;
up_SAT=10*Fj_eq;

dX = zeros(3,1);
dX(1)  = ((F/Vr)*(CA_0-X(1)))-(X(1)*K_0*exp(-E/(R*X(2))));
dX(2)  = ((F/Vr)*(T_0-X(2)))-((Lambda*X(1)*K_0*exp(-
E/(R*X(2))))/(Ro*Cp))-((U*Aj*(X(2)-X(3)))/(Vr*Ro*Cp));
dX(3)  = (min(max((Fj+v),0),up_SAT))*((Tc_in-X(3))/Vj) +
((U*Aj*(X(2)-X(3)))/(Vj*Roj*Cj));

end
```

A.4.2 Stabilizing CSTR by Sontag’s Stabilizer

```
clc
close all
CA_percentage=1.05;
Tr_percentage=0.95;
Tj_percentage=1.05;
time_order=4.7;

CA_eq = 1.6020; Tr_eq = 328.5763;Tj_eq = 310.2527;
```

```
X0 =
[CA_percentage*CA_eq;Tr_percentage*Tr_eq;Tj_percentage*Tj_eq];
X_eq=[CA_eq;Tr_eq;Tj_eq];
time=10^time_order;

options = odeset('RelTol',1e-4,'AbsTol',[1e-4 1e-4 1e-5]);
[T,X] = ode23tb(@CSTR2_Sontag,[0 time],X0,options);

figure
whitebg('w')
plot(T,X(:,1),'--',T,X(:,2),'--',T,X(:,3),'--')
legend('Reactanc Concentration','Reactant Temperature','Jacket
Temperature')
Grid on


figure
plot(T,X(:,1),'r',T,CA_eq,'b','LineWidth',1.2)
xlabel('Time')
legend('Reactant Concentration','Equilibrium Value')
grid on

figure
plot(T,X(:,2),'r',T,Tr_eq,'b','LineWidth',1.2)
xlabel('Time')
legend('Reactant Temperature','Equilibrium Value')
grid on

figure
plot(T,X(:,3),'r',T,Tj_eq,'b','LineWidth',1.2)
xlabel('Time')
legend('Jacket Temperature','Equilibrium Value')
grid on
```

A.5 CHECKING CLF CONDITION IN TERMS OF a(y) AND b(y)

```
close all
clc
%---syms CA_0 Lambda E Cp Cj F U Vj------------------------------
%---K_0 R Ro Roj Tc_in Vr Aj T_0 Fj------------------------------
syms Y1 Y2 Y3
CA_0 = 8.01; Lambda = - 69.71*10^6; E = 69.71*10^6;
Cp = 3137; Cj = 4183; F = 4.377*10^-3 ; U = 851;
Vj = 10.1; K_0 = 20.75*10^6; R = 8314;
Ro = 801; Roj = 1000; Tc_in = 294;
```

```
Vr = 102; Aj = 101; T_0 = 294;
Fj=0.0232;

P=eye(3,3)+[500,1,1;1,1,1;1,1,0]
eig(P)
Y=[Y1;Y2;Y3];

FF=[((F/Vr)*(CA_0-Y1))-(Y1*K_0*exp(-E/(R*Y2)));
   ((F/Vr)*(T_0-Y2))-((Lambda*Y1*K_0*exp(-E/(R*Y2)))/(Ro*Cp))-
(U*Aj*(Y2-Y3)/(Vr*Ro*Cp));
   (U*Aj*(Y2-Y3))/(Vj*Roj*Cj)];

GG=[0;0;(1/Vj)*(Tc_in-Y3)];

a=2*Y'*P'*FF;
b=2*Y'*P'*GG;

%---Evaluating a(y) At the Roots of b(y)------------------------
a_y02=subs(a,{Y1,Y2,Y3},{Y1,Y2,294});
a_y03=subs(a,{Y1,Y2,Y3},{-Y2-Y3,Y2,Y3});

figure
ezsurf(a_y02,[10^-6 10^6 10^-6 10^6])
grid on

figure
ezsurf(a_y03,[10^-6 10^6 10^-6 10^6])
grid on
```

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