Stability Analysis of a Non Adiabatic Continuous Stirred Tank Reactor

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Abstract

Chemical reaction systems can exhibit rather complex and interesting dynamic behaviour. The stability characteristics of a non-adiabatic continuous stirred tank reactor (CSTR) in which a simple exothermic conversion reaction occurs has been investigated. A dynamic model of the CSTR was developed from material and energy conservation laws applied to the reactor. The model which is a pair of ordinary differential equations (ODEs) was then transformed to a dimensionless ODE pair which constituted an autonomous system. Linear stability analysis was carried out. Results of steady state analysis indicate that the system exhibited steady state multiplicity with three steady states identified. Results obtained from carrying out linear stability analysis indicate that the high and low temperature steady states were a stable node and stable focus respectively. These steady states were stable while the intermediate temperature steady state was a saddle point hence it is unstable. The former can therefore be used for design purposes while the later cannot be utilised.

Keywords: **Steady state, Stability, Eigenvalue, Dynamics, Multiplicity, Jacobian**

Nomenclature
Concentrations:
A   Concentration of chemical species A ($kmol/m^3$)
B   Concentration of chemical species B ($kmol/m^3$)
H   Concentration of chemical species H ($kmol/m^3$)
X   Concentration of chemical species X ($kmol/m^3$)
Y   Concentration of chemical species Y ($kmol/m^3$)
Z   Concentration of chemical species Z ($kmol/m^3$)
Non dimensionless variables:
a   non dimensionless concentration of chemical species A
b   non dimensionless concentration of chemical species B
u   non dimensionless temperature
τ non dimensionless time
Others:
A_t Heat transfer area (m^2)
C_p Specific heat capacity of reaction mixture ($J/kg.K$)
e eigenvalues of Jacobian evaluated at steady state
I identity matrix
J Jacobian
k_i reaction rate constant ($1/s$)
K_u kinetic parameter
q Volumetric flowrate (m^3/s)
r reaction rate ($mol/m^3.s$)
U heat transfer coefficient between cooling coil and reactor content ($W/m^2.K$)
T reaction temperature (K)
V reactor volume (m^3)

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Subscripts:

c	coolant
f	feed conditions
o	reference conditions
s	steady state

Greek letters:

α	non dimensional parameter
β	non dimensional parameter
γ	extent of cooling
δ	heat of reaction intensity
ρ	density of liquid reaction mixture
λ	non dimensional parameter
ξ	vector of perturbations from steady state
ΔH	heat of reaction
θ	reactor residence time

1.0   Introduction

There has been a lot of interest in the problem of chemical reactor stability over the past three decades [1-5]. Recently, a lot of attention has been given to the various behaviours exhibited by chemical reaction systems. These behaviours include oscillating pH profiles, Turing and other patterns, symmetry breaking and pattern concatenation [6-12]. Instability in chemical reaction systems also referred to as chemical chaos exist in many aspects of the physical world [13]. Some concrete and definable examples of chemical chaos can be found in oscillating chemical reactions. One common example of such a reaction is the Belousov-Zhabotinskii reaction in chemistry [14]. The oscillatory behaviour observed for the BZ reaction can change from periodic to chaotic by simply changing the rate at which reactants are fed into the system. The BZ reaction has many variations but the most common involves the oxidation of organic materials that are easily brominated in an acidic medium. An example is the oxidation of malonic acid by bromate in acid environment catalysed by the redox couple Ce^{3+}/Ce^{4+}. For this case, the colour of the reacting mixture periodically changes from yellow to colourless and back to yellow. The chemistry of the BZ reaction is rather complex because of the presence of many kinetic steps, which makes it somewhat difficult to model [15]. Many kinetics steps have been proposed in the literature but the one outlined below known as the Oregonator was developed by researchers at the University of Oregon [14].

$$A + Y + 2H \xrightarrow{k_1} X + P \tag{1}$$

$$X + Y + H \xrightarrow{k_2} 2P \tag{2}$$

$$A + X + H \xrightarrow{k_3} 2X + 2Z \tag{3}$$

$$2X \xrightarrow{k_4} A + P + H \tag{4}$$

$$B + Z \xrightarrow{k_5} fY \tag{5}$$
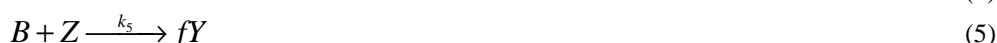
Based on the kinetic steps of (1) to (5), the BZ reaction system is described by the following equations.

$$\frac{dX}{dt} = k_1 AH^2Y - k_2 HXY + k_3 AHX - 2k_4 X^2 \tag{6}$$

$$\frac{dY}{dt} = -k_1 AH^2Y - k_2 HXY + fk_5 BZ \tag{7}$$

$$\frac{dZ}{dt} = 2k_3 AHX - k_5 BZ \tag{8}$$

By making the following transformations, the equation set of (6) to (8) can be presented in dimensionless form as follows.

$$x = \frac{X}{X_o} \qquad y = \frac{Y}{Y_o} \qquad z = \frac{Z}{Z_o} \qquad a = \frac{A}{A_o} \qquad b = \frac{B}{B_o} \qquad \tau = \frac{t}{t_o}$$

$$\alpha \frac{dx}{d\tau} = \mu ay - xy + ax - x^2 \tag{9}$$

$$\beta \frac{dy}{d\tau} = -\mu a y - xy + \delta b z \tag{10}$$

$$\frac{dz}{d\tau} = ax - bz \tag{11}$$

x, y and *z* are the dimensionless concentrations of species X, Y and Z respectively while τ is the dimensionless time.

Where: $\quad \alpha = \dfrac{k_5 B_o}{k_3 HA_o} \qquad \beta = \dfrac{2k_4 k_5 B_o}{k_2 k_3 H^2 A_o} \qquad \mu = \dfrac{2k_1 k_4}{k_2 k_3} \qquad \delta = 2f$

The subscripts (o) indicate reference conditions and are defined as follows.

$$X_o = \frac{k_3 HA_o}{2k_4} \qquad Y_o = \frac{k_3 A_o}{k_2} \qquad Z_o = \frac{(k_3 HA_o)^2}{k_4 k_5 B_o} \qquad t_o = \frac{1}{k_5 B_o}$$

Another example of a chemical reaction system that exhibits instability and chaotic behaviour is the autocatalator. This is a slightly simpler but similar reaction involving three variables hence it is referred to as the three-variable autocatalator [16]. Autocalators are usually isothermal reactions that proceed in closed systems. For the autocatalytic reaction system, a molecule of one of the chemical species involved in the reaction produces more molecules of itself in the course of the reaction. This provides internal feedback for the system and leads to robust dynamic behaviour. One of the chemical reaction systems exhibiting rich dynamic behaviour is the isothermal cubic autocatalator introduced by Gray and Scott [2]. This reaction system is presented in the terms of the following kinetic steps.

$$P \xrightarrow{k_o} A \tag{12}$$

$$A \xrightarrow{k_1} B \tag{13}$$

$$A + 2B \xrightarrow{k_2} 3B \tag{14}$$

$$B \xrightarrow{k_4} C \tag{15}$$

Based on the kinetic steps of (12) to (15), the equations describing the concentrations of species A and B are:

$$\frac{dA}{dt} = -k_0 P - k_1 A + k_2 AB^2 \tag{16}$$

$$\frac{dB}{dt} = k_1 A + k_2 AB^2 - k_3 B \tag{17}$$

By making the following transformations, equations (16) and (17) can be presented in dimensionless form as follows.

$$a = \frac{A}{A_o} \qquad b = \frac{B}{B_o} \qquad \tau = \frac{t}{t_o}$$

$$\frac{da}{d\tau} = \mu - K_u a - ab^2 \tag{18}$$

$$\frac{db}{d\tau} = K_u a + ab^2 - b \tag{19}$$

a and *b* are the dimensionless concentrations of species A and B respectively while τ is the dimensionless time.

Where: $\quad \mu = \left(\dfrac{2k_0^2 k_2}{k_3^3} \right)^{1/2} [P]_o \qquad K_u = \dfrac{k_1}{k_3}$

The subscripts (o) indicate reference conditions and are defined as follows.

$$A_o = \sqrt{\frac{k_3}{k_2}} \qquad B_o = \sqrt{\frac{k_3}{k_2}} \qquad t_o = \frac{1}{k_3}$$

The concept of stability is one of the key aspects of dynamical systems. Consider a system of nonlinear ordinary differential equations (ODEs) written as:

$$\frac{dy_i}{d\tau} = f_i(y_1, y_2, .., y_n) \qquad i = 1, 2, ..., n \tag{20}$$

Equation (20) can be written in vector form as:

$$\frac{d\overline{y}}{d\tau} = \overline{f}(\overline{y})$$ (21)

Where

$$\overline{y} = [y_1, y_2, ..., y_n] \qquad \overline{f} = [f_1, f_2, ..., f_n]$$

Since the functions f_i depend only on $\overline{y}$ and not explicitly on t, the ODE system described by Equation (20) is referred to as an autonomous system. A constant vector $\overline{y}_s$ for which Equation (22) is true is called a steady state or an equilibrium point.

$$f(\overline{y}_s) = 0$$ (22)

If more than one $\overline{y}_s$ satisfies Equation (22), then multiple steady states will exist. When an initial condition is provided such as, $\overline{y}(0) = \overline{y}_s$ the solution to the ODE set will be $\overline{y}(t) = \overline{y}_s \qquad \forall t \geq 0$. For this case, the solution is often presented as a trajectory which is a nonlinear plot of $\overline{y}(t)$ as a function of time in the n-dimensional phase space of $\overline{y}$. Every steady state is represented by a specific point in the phase space and every point in the phase space is a potential initial condition. With the foregoing in mind, the following definitions can be presented.

Definition 1: A steady state or equilibrium point $\overline{y}_s$ of the ODE set of Equation (21) is said to be stable if all eigenvalues of the Jacobian J_s evaluated at $\overline{y}_s$ have real and negative values. The Jacobian is the matrix of partial derivatives of the ODE set of equation (21) evaluated with respect to the state vector variables $\overline{y}$. The Jacobian of the ODE set of equation (21) is given as:

$$J = \begin{pmatrix} \frac{\partial f_1}{\partial y_1} & \frac{\partial f_1}{\partial y_2} & \cdots & \frac{\partial f_1}{\partial y_n} \\ \frac{\partial f_2}{\partial y_1} & \frac{\partial f_2}{\partial y_2} & & \frac{\partial f_2}{\partial y_n} \\ \vdots & \vdots & & \vdots \\ \frac{\partial f_n}{\partial y_1} & \frac{\partial f_n}{\partial y_2} & \cdots & \frac{\partial f_1}{\partial y_n} \end{pmatrix}$$

If the Jacobian is evaluated at the steady state, it is expressed as:

$$J_s = \begin{pmatrix} \frac{\partial f_1}{\partial y_1} & \frac{\partial f_1}{\partial y_2} & \cdots & \frac{\partial f_1}{\partial y_n} \\ \frac{\partial f_2}{\partial y_1} & \frac{\partial f_2}{\partial y_2} & & \frac{\partial f_2}{\partial y_n} \\ \vdots & \vdots & & \vdots \\ \frac{\partial f_n}{\partial y_1} & \frac{\partial f_n}{\partial y_2} & \cdots & \frac{\partial f_1}{\partial y_n} \end{pmatrix}_s$$

The steady state or equilibrium point is unstable if at least one of the eigenvalues of the Jacobian evaluated at the steady state has a positive real value. The eigenvalues of the Jacobian must satisfy the condition:

$$|J - eI| = 0$$ (23)

e represents the eigenvalues of the Jacobian while I is an identity matrix
For a 2-dimensional autonomous system, equation (23) results in:

$$e^2 - (trJ)e + |J| = 0$$ (24)

Thus, the two eigenvalues are given by:

$$e_{1,2} = \frac{1}{2}\left[trJ \pm \sqrt{(trJ)^2 - 4|J|}\right]$$ (25)

Where trJ represents the trace of the Jacobian given as the sum of the off-diagonal elements of the Jacobian while $|J|$ represents the determinant of the Jacobian.

For the case where both eigenvalues e_1 and e_2 are real, the term under the square root sign must satisfy the condition:

$$(trJ)^2 - 4|J| > 0 \qquad\qquad (trJ)^2 > 4|J|$$

The eigenvalues e_1 and e_2 are both negative if and only if their sum is negative and their product is positive, i.e.,

$$e_1 + e_2 < 0 \tag{26}$$

$$e_1 e_2 > 0 \tag{27}$$

Combining equations (25) and (26) results in:

$$trJ < 0 \tag{28}$$

Combining equations (25) and (27) results in:

$$|J| > 0 \tag{29}$$

Definition 2: Regardless of whether the eigenvalues of the Jacobian are real or complex, the steady state under consideration is considered stable if and only if the condition

$$trJ < 0 \text{ and } |J| > 0$$

are satisfied simultaneously. Table 1 gives a summary of the type and stability character resulting from the eigenvalues of the Jacobian evaluated at the steady state.

**Table 1:** Summary of steady state type and character

Eigenvalues	Steady state type	Stability character
Real and negative	Stable node	Asymptotically stable
Real and positive	Unstable node	Unstable
Real, equal and negative (Symmetric Jacobian)	Stable proper node	Asymptotically stable
Real, equal and positive (Symmetric Jacobian)	Unstable proper node	Unstable
Real, equal and negative (Unsymmetric Jacobian)	Stable improper node	Asymptotically stable
Real, equal and positive (Unsymmetric Jacobian)	Unstable improper node	Unstable
Real and unequal (opposite signs)	Saddle point	Unstable
Complex with positive real parts	Unstable focus (spiral source)	Unstable
Complex with negative real parts	Stable focus (spiral sink)	Asymptotically stable
Complex with zero real parts (purely imaginary roots)	Center	Marginally stable

Of the several types of reactors encountered in the chemical process industry, the continuous stirred tank reactor (CSTR) is the most commonly used because it is the most amenable to control action [17,18]. The flow of reactants inside the reactor is smooth and continuous [17,19,20]. The concentrations and temperature of the species in the reactor do not vary with position and these have the same values as that in the effluent steam [21].

In this work, we consider the stability analysis of a nonadiabatic CSTR in which a simple reaction for the conversion of a single reactant to a single product occurs. This relatively simple chemical reaction system can exhibit rather complex and interesting dynamic behaviour. The specific objectives of the study include determining the steady state(s) of the system and obtaining the stability criteria for which the steady state(s) is(are) either stable or unstable to small perturbations.

2. Non Adiabatic CSTR Model

The non-adiabatic CSTR with single input and single output in which a simple conversion reaction takes place is shown in Figure 1.
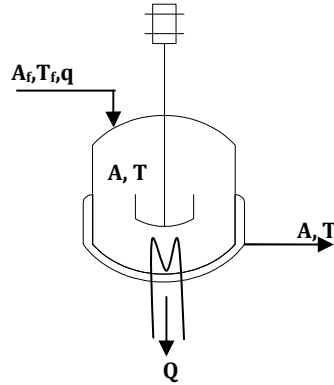
Figure 1: Schematic of non-adiabatic CSTR

The reaction occurring in the reactor is described by the simple chemical equation expressed as:

$$A \xrightarrow{k} P \qquad \text{(Exothermic)}$$

The CSTR model formulated from transient mass and energy balance is given by the following pair of ordinary differential equations (32) and (33).

$$\frac{dA}{dt} = \frac{q}{V}(A_f - A) - r \tag{30}$$

For a first order reaction:

$$r = kA \tag{31}$$

The material balance for A becomes:

$$\frac{dA}{dt} = \frac{q}{V}(A_f - A) - kA \tag{32}$$

The energy balance about the reactor gives:

$$V\rho C_p \frac{dT}{dt} = q\rho C_p(T_f - T) - UA_t(T - T_c) + V(-\Delta H)kA \tag{33}$$

The ODE pair of (32) and (33) has the following initial conditions:

$$A = A_o; \quad T = T_o \quad \text{at} \quad t = 0$$

By making the following transformations, equations (32) and (33) can be presented in dimensionless form as follows.

$$a = \frac{A}{A_f} \qquad u = \frac{T}{T_f} \qquad u_c = \frac{T_c}{T_f} \qquad \tau = \frac{t}{\theta} \qquad \theta = \frac{V}{q}$$

$$\frac{da}{d\tau} = 1 - a - \lambda a \tag{34}$$

$$\frac{du}{d\tau} = 1 - u - \gamma(u - u_c) + \delta a \tag{35}$$

a is the dimensionless concentration of A, u is the dimensionless temperature while τ is the dimensionless time. Where:

$$\lambda = k\theta \qquad \gamma = \frac{UA_t\theta}{V\rho C_p} \qquad \delta = \frac{(-\Delta H)kA_f\theta}{\rho C_p T_f}$$

2.1. Linearized Stability Analysis

The dimensionless ODE pair of (34) and (35) is an autonomous system with the following initial conditions:

$$a = a_o; \quad u = u_o \quad \text{at} \quad \tau = 0$$

$$\frac{da}{d\tau} = 1 - a - \lambda a = f_1(a, u) \tag{34}$$

$$\frac{du}{d\tau} = 1 - u - \gamma(u - u_c) + \delta a = f_2(a, u) \tag{35}$$

The steady state(s) of the autonomous system is (are) obtained by setting both time derivatives to zero.

From (34): $\qquad \dfrac{da}{d\tau} = 0 = 1 - a_s - \lambda a_s$

On resolving:

$$a_s = \frac{1}{1 + \lambda} \tag{36}$$

From (35): $\qquad \dfrac{du}{d\tau} = 0 = 1 - u_s - \gamma(u_s - u_c) + \delta a_s$

On resolving:

$$u_s = \frac{1 + \gamma u_c + \delta a_s}{1 + \gamma} \tag{37}$$

On substituting for a_s:

$$u_s = \frac{1 + \gamma u_c + \frac{\delta}{1+\lambda}}{1 + \gamma} \tag{38}$$

Thus the unique steady state is:

$$a_s = \frac{1}{1 + \lambda} \quad \text{and} \quad u_s = \frac{1 + \gamma u_c + \frac{\delta}{1+\lambda}}{1 + \gamma}$$

In order to determine whether or not the steady state is asymptotically stable or otherwise, we consider the following linearized system given as:

$$\frac{da}{d\tau} = J\xi \tag{39}$$

Where the vector of perturbations from the steady state (a_s, u_s) is given as:

$$\xi = \begin{bmatrix} a - a_s \\ u - u_s \end{bmatrix} \tag{40}$$

The Jacobian evaluated at the steady state is given as:

$$J_s = \begin{pmatrix} \left.\frac{\partial f_1}{\partial a}\right|_s & \left.\frac{\partial f_1}{\partial u}\right|_s \\ \left.\frac{\partial f_2}{\partial a}\right|_s & \left.\frac{\partial f_2}{\partial u}\right|_s \end{pmatrix} \tag{41}$$

The partial derivatives are evaluated from the autonomous system represented by equations (34) and (35). Hence:

$$J_s = \begin{pmatrix} -(1+\lambda) & 0 \\ \delta & -(1+\gamma) \end{pmatrix} \tag{42}$$

For the Jacobian, the trace and determinant are respectively given as:

$$trJ = -(1+\lambda) - (1+\gamma) = -(\lambda + \gamma)$$
$$trJ = -(\lambda + \gamma)$$
$$|J| = (1+\lambda)(1+\gamma) \tag{43}$$

For the steady state to be stable to small perturbations, it must satisfy the conditions below simultaneously.

$$trJ < 0 \quad \text{and} \quad |J| > 0$$

From the result obtained, the trace of the Jacobian is: $trJ = -(\lambda + \gamma)$.

Since the parameters λ and γ are both positive, then it follows that the trace of the Jacobian is negative. Thus the first condition is satisfied.

In the same way, the determinant of the Jacobian i.e., $|J| = (1+\lambda)(1+\gamma)$ is positive as both parameters are positive.

Since the unique steady state simultaneously satisfies both criteria for stability, it follows that it is asymptotically stable. The criteria for stability for the autonomous system under consideration are thus:

- $-(\lambda + \gamma) < 0$ or $(\lambda + \gamma) > 0$
- $(1+\lambda)(1+\gamma) > 0$

Recalling that $\lambda = k\theta$ $\gamma = \dfrac{UA_t\theta}{V\rho C_p}$, both criteria can be transformed to obtain:

- $\left(k\theta + \dfrac{UA_t\theta}{V\rho C_p}\right) > 0$

- $\left[(1+k\theta) + \left(1 + \dfrac{UA_t\theta}{V\rho C_p}\right)\right] > 0$

2.2. Classification of Unique Steady State
The eigenvalue problem for the Jacobian is cast as follows:
$$|J - eI| = 0 \tag{44}$$

I is an identity matrix

$$|J - eI| = \begin{vmatrix} -(1+\lambda) - e & 0 \\ \delta & -(1+\gamma) - e \end{vmatrix} = 0 \tag{45}$$

The eigenvalues of the Jacobian evaluated at the unique steady state are thus:
$$e_1 = -(1+\lambda)$$
$$e_2 = -(1+\gamma)$$

Since the parameters λ and γ are both positive and real, it follows that both eigenvalues are real and negative. Following the classification criteria of Table 1, it is seen that the unique steady state is a stable node whose stability character is "asymptotically stable".

3.0 Case study: Single, first-order exothermic irreversible reaction in a non-Adiabatic CSTR

Exothermic reactions are one of the most interesting chemical reaction systems to study because of potential existence of multiple steady-states. Consider a CSTR with a single, first-order exothermic irreversible reaction occurring in a non-adiabatic CSTR.

$$A \xrightarrow{k} B \qquad \text{(Exothermic)}$$

The first order rate of reaction is given as:

$$r = k_o \exp\left(\dfrac{-E}{RT}\right)A \tag{46}$$

For the CSTR shown in Figure 1, the following assumptions were made in developing a model for the reaction.

- Perfect mixing
- Constant density and volume
- Constant parameter values
- The cooling jacket temperature can be directly manipulated. This removes the need to carry out an energy balance around the jacket.

The material and energy balance equations for A becomes:

$$\dfrac{dA}{dt} = \dfrac{q}{V}(A_f - A) - r \tag{47}$$

$$V\rho C_p \frac{dT}{dt} = q\rho C_p (T_f - T) - UA_t(T - T_c) + V(-\Delta H)r \tag{48}$$

The ODE pair of (47) and (48) has the following initial conditions:

$$A = A_o; \quad T = T_o \quad \text{at} \quad t = 0$$

The pair of equations (49) and (50) also constitutes the modelling equations given as:

$$f_1(A,T) = \frac{dA}{dt} = \frac{q}{V}(A_f - A) - k_o \exp\left(\frac{-E}{RT}\right)A \tag{49}$$

$$f_2(A,T) = \frac{dT}{dt} = \frac{q}{V}(T_f - T) - \frac{UA_t}{V\rho C_p}(T - T_c) + \frac{(-\Delta H)}{\rho C_p}r \tag{50}$$

3.1. Steady state solution:

The steady state solution is obtained when both time derivatives of equations (49) and (50) are set to zero i.e.

$$f_1(A,T) = \frac{dA}{dt} = 0; \quad f_2(A,T) = \frac{dT}{dt} = 0$$

The values of parameters used in obtaining the steady state solution are presented in Table 2.

Table 2: Parameter values for steady state solution [22]

Solution parameter	Value	Units
V	1	m^3
q	1	m^3/h
T_f	25	^oC
T_c	25	^oC
E	49584	$kJ/kmol$
k_o	34930800	$1/h$
A_f	10	$kmol/m^3$
$(-\Delta H)$	24953	$kJ/kmol$
ρC_p	2093	$kJ/^oCm^3$
UA_t	628	$kJ/h\,^oC$

As with most numerical solution methods, the initial condition of a variable determines the value to which that variable will converge to during solution. For this case study, three initial conditions were chosen viz:

- Initial condition A: This is the low temperature, high concentration and low conversion condition characterised by the variable values ($A = 9kmol/m^3$ and $T = 27^oC$)

This initial condition led to the following steady state solution tagged the low temperature steady state:

$$\begin{bmatrix} A_s \\ T_s \end{bmatrix} = \begin{bmatrix} 8.56 \\ 38.1 \end{bmatrix}$$

- Initial condition B: This is the intermediate temperature, concentration and conversion condition characterised by the variable values ($A = 5kmol/m^3$ and $T = 77^oC$)

This initial condition led to the following steady state solution tagged the intermediate temperature steady state:

$$\begin{bmatrix} A_s \\ T_s \end{bmatrix} = \begin{bmatrix} 5.52 \\ 66.1 \end{bmatrix}$$

- Initial condition C: This is the high temperature, low concentration and high conversion condition characterised by the variable values ($A = 1kmol/m^3$ and $T = 177^oC$)

This initial condition led to the following steady state solution tagged the high temperature steady state:

$$\begin{bmatrix} A_s \\ T_s \end{bmatrix} = \begin{bmatrix} 2.36 \\ 95.1 \end{bmatrix}$$

These are the only possible solutions as other initial conditions did not lead to any other solutions for the given set of parameter values.

3.2 Linearized Stability Analysis and classification of steady states

By making the following transformations, equations (39) and (40) can be presented in dimensionless form as follows.

$$a = \frac{A}{A_f} \qquad u = \frac{T}{T_f} \qquad u_c = \frac{T_c}{T_f} \qquad \tau = \frac{t}{\theta} \qquad \theta = \frac{V}{q}$$

$$\frac{da}{d\tau} = 1 - a - \lambda a \tag{51}$$

$$\frac{du}{d\tau} = 1 - u - \gamma(u - u_c) + \delta a \tag{52}$$

a is the dimensionless concentration of A, u is the dimensionless temperature while τ is the dimensionless time.

Where: $\lambda = k'\theta \qquad \gamma = \dfrac{UA_t\theta}{V\rho C_p} \qquad \delta = \dfrac{(-\Delta H)k'A_f\theta}{\rho C_p T_f}$

The ODE pair of (41) and (42) is an autonomous system with the following initial conditions: $a = a_o; \quad u = u_o \quad$ at $\quad \tau = 0$

$$\frac{da}{d\tau} = 1 - a - \lambda a = f_1(a,u) \tag{53}$$

$$\frac{du}{d\tau} = 1 - u - \gamma(u - u_c) + \delta a = f_2(a,u) \tag{54}$$

In order to determine the stability of the autonomous system, we consider the following linearized system given as:

$$\frac{da}{d\tau} = J\xi \tag{55}$$

Where the vector of perturbations from the steady state (a_s, u_s) is given as:

$$\xi = \begin{bmatrix} a - a_s \\ u - u_s \end{bmatrix} \tag{56}$$

The Jacobian evaluated at the steady state is given as:

$$J_s = \begin{pmatrix} \left.\frac{\partial f_1}{\partial a}\right|_s & \left.\frac{\partial f_1}{\partial u}\right|_s \\ \left.\frac{\partial f_2}{\partial a}\right|_s & \left.\frac{\partial f_2}{\partial u}\right|_s \end{pmatrix} \tag{57}$$

The partial derivatives are evaluated from the autonomous system represented by equations (51) and (52).

Hence: $J_s = \begin{bmatrix} -\dfrac{q}{V} - k & -Ak \\ \dfrac{(-\Delta H)k}{\rho C_p} & -\dfrac{q}{V} + \dfrac{(-\Delta H)Ak}{\rho C_p} - \dfrac{UA_t}{V\rho C_p} \end{bmatrix}_s \tag{58}$

Inputting the parameter values in Table 2 into the Jacobian, the eigenvalues were calculated for each initial condition. The results obtained as presented as follows.

- Initial condition A: $\begin{bmatrix} A_s \\ T_s \end{bmatrix} = \begin{bmatrix} 8.61 \\ 38.5 \end{bmatrix}$

  For this operating point, the eigenvalues are respectively:
  $\lambda_1 = -0.91$ and $\lambda_2 = -0.50$

- Initial condition B: $\begin{bmatrix} A_s \\ T_s \end{bmatrix} = \begin{bmatrix} 5.55 \\ 66.3 \end{bmatrix}$

  For this operating point, the eigenvalues are respectively:

$$\lambda_1 = -0.85 \text{ and } \lambda_2 = 0.50$$

- Initial condition C: $\begin{bmatrix} A_s \\ T_s \end{bmatrix} = \begin{bmatrix} 2.41 \\ 95.3 \end{bmatrix}$

  For this operating point, the eigenvalues are respectively:

$$\lambda_1 = -0.78 + 0.93i \text{ and } \lambda_2 = -0.78 - 0.93i$$

Based on the classification criteria presented in Table 1, the multiple steady states are thus classified.

- Initial condition A: Real and negative eigenvalues implies that this steady state is a stable node which is asymptotically stable.
- Initial condition B: Real and unequal eigenvalues with opposite signs implies that this steady state is a saddle point which is inherently unstable.
- Initial condition C: Complex eigenvalues with negative real parts implies that this steady state is a stable focus or spiral sink which is stable.

The phase space plot showing the coexistence of all steady state is shown in Figure 2.
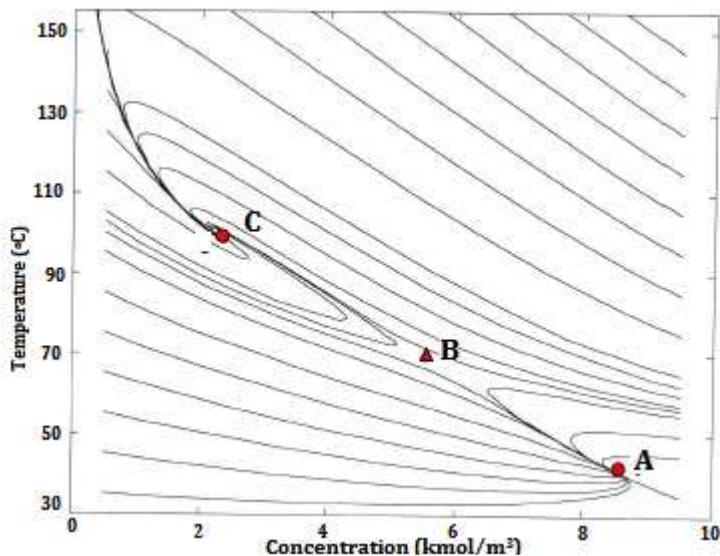
Figure 2: Phase plane plot for three steady states coexisting A (stable node), B(saddle point) and C (stable focus)

4.   Conclusion

In this work, the concept of dynamical systems and how it applies to chemical reactor stability has been introduced. The case for investigation was a non-adiabatic continuous stirred tank reactor in which a simple exothermic conversion reaction takes place. The exothermic reaction exhibits steady state multiplicity with three steady states existing. The low, intermediate and high temperature steady states are characterised as a stable node, saddle point and stable focus respectively. Both the low temperature and high temperature steady states were stable and can be used for design purposes. The intermediate temperature steady state was found to be unstable and cannot be utilised for design purposes.

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