CONCENTRATION OSCILLATIONS IN HETEROGENEOUS CATALYSTS

A Thesis

Presented to the

Faculty of the Department of

Chemical Engineering at the

University of Houston.

In partial fulfillment of the requirements

for the degree of Master of Science in Chemical

Engineering.

By

Constantine Andrew Pikios

December 1975

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Abstract

The purpose of this study was to examine whether it is possible for concentration oscillations to occur in the case of the isothermal reaction $A(g) + B(g) \longrightarrow AB$, which is taking place on a catalytic foil. By assuming a Langmuir-Hinshelwood kinetic mechanism in which the energy of activation for the final step depends linearly on the coverage by adsorbed B(g), we were able to derive the differential equations for the net rates of adsorption of A(g) and B(g). The necessary and sufficient conditions for stability were derived for the special case $k_1[A]=k_2[B]$. In addition, uniqueness criteria were derived for various ranges of the kinetic parameters. Numerical integration of the dynamic equations proved the possible existence of sustained oscillations in the case of a unique, unstable steady state, with a period between 11-17 seconds. However, we have not been able to find any examples of limit cycles for a case in which multiple steady states exist. Application of bifurcation theory did not lead to the finding of limit cycles in the case of multiple steady states.

TABLE OF CONTENTS

Chapter

LIST OF FIGURES

LIST OF TABLES

CHAPTER I

Introduction

During the past few years a number of publications have reported phenomena involving catalytic pellets, wires and foils, which cannot be explained by the already existing dynamic models of lumped and distributed parameter systems.

The puzzling behavior observed during these experiments was temperature and composition oscillations in isothermal and nonisothermal heterogeneous catalytic systems. For example, Wicke and coworkers [1] observed concentration and temperature oscillations with amplitudes up to 60 °C and periods from minutes up to hours during the oxidation of hydrogen on a 8 mm spherical, 0.4% Pt on silica-alumina catalytic pellet. The causes for these low frequency oscillations and their mechanism is unknown and the existing dynamic models are incapable of predicting this phenomenon. Wicke attempted to explain the periodicity by assuming that "it originates from particular reaction mechanisms which produce long time periodic changes in the nature of the active catalyst surface" [1]. Another possibility might be the effect of temperature on the adsorption and desorption rates of the reacting species [6].

For the isothermal case, Wicke and coworkers [1] investigated the CO oxidation over a 3X3 mm cylindrical, 0.3% Pt on γ-Al_2O_3 catalytic pellet. The reaction rate goes through a maximum with increasing concentration of the reactants (self-poisoning), because the strong chemisorption of CO inhibits the reaction rate at higher CO partial pressures. When this is the case, the reacting system may become unstable even under isothermal operating conditions. In fact, temperature and concentration oscillations do appear when the feed's temperature is below 250 °C. A mechanism explaining this phenomenon has to be presented.

Hugo and Jakubith [3] have reported similar concentration oscillations during the isothermal oxidation of CO on a platinum gauze. They attributed the observed phenomenon to the existence of two types of adsorbed CO molecules.

Dauchot and Cakenberghe [4] experimented with the catalytic oxidation of CO -under isothermal conditions- on a thin platinum film evaporated on silica. Again, concentration oscillations were observed. They interpreted this phenomenon by postulating that the reaction mechanism shifts from an Eley-Rideal to a Langmuir-Hinshelwood type. When oxygen has been mostly adsorbed, the hot catalytic surface begins to cool down and CO is progressively adsorbed -with or without the contribution of an Eley-Rideal reaction. After an induction period the reaction starts and proceeds rapidly. The CO is eliminated by a Langmuir-Hinshelwood reaction, the hot resulting surface is again instantly covered with oxygen, and the cycle is repeated. They suggest that the interaction between the local surface temperature and concentration causes this oscillatory behavior.

McCarthy [19] has shown in his study of CO oxidation over supported Pt that the mechanism for this reaction is complex, with a two-step rate control (O_2 adsorption and gaseous CO reacting with adsorbed O_2). The observed rate-CO concentration behavior is, in fact, a competitive conspiracy of two distinct rate processes: (1) Chemisorption of O_2 upon a surface partially covered with CO, and (2) an Eley-Rideal-type reaction of gaseous CO with adsorbed O_2. In the region in which both rates are of comparable magnitude, isothermal limit cycling is observed. This suggests that the CO oxidation over supported Pt is not a unique reaction between surface adsorbed species, which would give rise to

$$R=k''*(O_2)*(CO_2)*(1+K(CO))^{-2}$$

because this equation is based on a model of a one-step rate control and, consequently, could not give rise to limit cycling.

Recently, Slinko and coworkers [5] have observed concentration oscillations during the isothermal oxidation of hydrogen on a nickel foil. They claim that these oscillations can be explained by a surface kinetics mechanism where the rate limiting step is the reaction between adsorbed hydrogen and adsorbed oxygen. In other words, they assume a Langmuir-Hinshelwood-type mechanism in which the rate constant for the limiting step depends on the surface coverage by oxygen. Their paper, however, does not contain any kinetic parameter values, or numerical simulations which demonstrate that the proposed kinetic mechanism agrees with experimental results.

The main purpose of our research work has been to test the claim of Slinko and coworkers [5] by investigating the stability characteristics of the same surface kinetics mechanism. The question is asked whether there exist parameter values for which the ordinary differential equations representing the rates of adsorption of the gaseous reactants on the catalytic surface exhibit oscillatory behavior. In other words, we are attempting to determine kinetic parameters for which oscillatory solutions exist.

The kinetic scheme chosen for this study and the basic assumptions are expounded in the next chapter along with the mathematical equations representing the physical model. One cannot avoid noticing the similarity between our differential equations and those of Poore and coworkers [9,10], who investigated the stability characteristics of a continuously stirred tank reactor (CSTR). The methodology shown in the work of Poore and coworkers [9,10] is similar to the one followed in our study, although our differential equations are considerably more complicated. As result of this complexity, some of the mathematical techniques used by Poore to predict the direction of bifurcation of the periodic orbits as one of the parameters is varied cannot be employed here.

The fact that existing dynamic models do not predict the experimental phenomena mentioned in the above publications is an indication that certain important chemical processes have not been taken into account. What has been heretofore neglected is the inclusion of the adsorption capacity of the various reacting species on the catalytic surface. Elnashaie and Cresswell [7,8] have demonstrated that neglecting the dynamics of the adsorption-reaction-desorption process may produce a very oversimplified picture of the behavior and stability of catalytic pellets. One is inclined to believe that what is needed is the use of more sophisticated dynamic models than those used up until now. Such models would not only represent more accurately the actual physical situation, but would also be more helpful for design and industrial purposes. It is hoped that the present study is a small step in this direction.

CHAPTER II

Here, we discuss the following topics: First, the heterogeneous catalytic mechanism postulated for the general chemical reaction

$$A(g) + B(g) \longrightarrow AB$$

Second, the basic assumptions accompanying the kinetic mechanism chosen for this reaction. Third, the derivation of the differential equations for the rates of chemisorption of reactants A(g) and B(g) on the catalytic surface; and, fourth, the form of the steady state equations.

IIa] Postulated kinetic mechanism

Suppose that the chemical reaction

$$A(g) + B(g) \longrightarrow AB$$

takes place on a catalytic surface. The mechanism assumed for this reaction consists of the following kinetic steps:

$$A(g) + [S] \longrightarrow (A\text{-}S)$$

$$B(g) + [S] \longrightarrow (B\text{-}S)$$

$$(A\text{-}S) + (B\text{-}S) \longrightarrow AB + 2[S]$$

where [S] denotes an active surface site, while (A-S) and (B-S) denote the adsorbed reactants A(g) and B(g), respectively. The mechanism for which both reactants have to be adsorbed on the surface for the final product to be formed is known as a Langmuir-Hinshelwood mechanism.

Instead of a Langmuir-Hinshelwood we could have assumed an Eley-Rideal mechanism. In the latter, only one reactant has to be chemisorbed on the catalytic surface while the other has to strike the adsorbate from the gas phase in order to form a bond between them. For the reaction chosen in our study, an Eley-Rideal mechanism consists of the following kinetic steps:

$$A(g) + [S] \longrightarrow (A\text{-}S)$$

$$(A\text{-}S) + B(g) \longrightarrow AB + [S]$$

In the present work, however, the mechanism postulated for the reaction was a Langmuir-Hinshelwood rather than an Eley-Rideal-type, because the mathematical analysis is less complicated. Hopefully, in some later time an analysis will be attempted assuming an Eley-Rideal mechanism, or a hybrid of an Eley-Rideal and Langmuir-Hinshelwood. In either case, analytical results should be compared with experimental to decide whether the kinetic model is realistic.

IIb] Basic assumptions

a) Let $\{S\}$ denote the number of active surface sites which are not occupied at time t. Then, the total number of active sites on the catalytic surface, L, is given by

$$L = \{S\} + \{A-S\} + \{B-S\}$$

where $\{A-S\}$ and $\{B-S\}$ denote the number of active sites occupied at time t by adsorbed A(g) and B(g), respectively. Then

$$\{S\} = L - \{A-S\} - \{B-S\}$$

and after dividing both sides by L

$$\zeta = 1-x-y$$

where

ζ: represents the fraction of active surface sites which are not occupied at time t.

x: represents the coverage of the catalytic surface with adsorbed A(g) at time t.

y: represents the coverage of the catalytic surface with adsorbed B(g) at time t.

b) For the kinetic mechanism

$$A(g) + [S] \longrightarrow (A\text{-}S)$$

$$B(g) + [S] \longrightarrow (B\text{-}S)$$

$$(A\text{-}S) + (B\text{-}S) \longrightarrow AB + 2[S]$$

we assume that the number of sites on the adsorbent is constant, and each site can adsorb one species only. All sites are identical but the activation energy for adsorption increases linearly with coverage due to induced heterogeneity: i.e., (i) there are lateral (repulsive) interactions between adsorbed molecules which are uniformly distributed over the available sites, or (ii) the adsorbate molecules by perturbation of the adsorbent surface, change the properties of the remaining free sites such that the activation energy increases with coverage. In our study we postulate that the adsorbed B(g), (B-S), changes the properties of the catalytic surface and the greatest influence is in the third step. In that case, the energy of this step depends on the coverage by adsorbed B(g)

$$E_3 = E_3^0 + \mu RTy \qquad (1)$$

where μ is the coefficient of heterogeneity of the catalytic surface. The above relation for the energy of activation of the adsorption process is identical to the one shown in the work of Slinko and coworkers [5]; its derivation and more extensive discussions can be found in the works of Brunauer et. al. [21], Aharoni and Tompkins [22], as well as Weber and Loučka [15].

The rate constant for the surface reaction is given by

$$k_3 = k_{30}\ e^{-E_3/RT} \qquad (2)$$

Because of (1), we can rewrite (2) as

$$k_3 = (\ k_{30}\ e^{-E_3^0\ /RT})\ e^{-\mu y} \qquad (3)$$

c) We assume that the reaction

$$A(g) + B(g) \longrightarrow AB$$

occurs under isothermal conditions. If this is the case, we can rewrite equ.(3) as

$$k_3 = k\ e^{-\mu y} \qquad (4)$$

where

$$k = k_{30}\ e^{-E_3^0/RT} \qquad (5)$$

Finally, assuming a first order rate dependence with respect to (A-S) and (B-S), the rate for the surface reaction is given by

$$r = k_3\ xy L^2 \qquad (6)$$

Because of (4), we can rewrite (6) as

$$r = k\ e^{-\mu y}\ xy L^2 \qquad (7)$$

IIc] Dynamic equations

The net rates of adsorption of A(g) and B(g) on the catalytic surface are given by the following nonlinear, coupled, ordinary differential equations:

$$\frac{dx}{dt} = K_1[A](1-x-y) - K_{-1}x - K_3^{\circ} e^{-\mu y} x y \equiv f_1(x,y) \qquad (8)$$

$$\frac{dy}{dt}=k_2[B](1-x-y)-k_{-2}y-k_3^0 e^{-\mu y}xy \equiv f_2(x,y) \qquad (9)$$

where [A] and [B] denote concentrations of A(g) and B(g), respectively, and

$$k_3^0 = kL$$

note that the above differential equations, although considerably more complicated, are similar to the equations appearing in the work of Poore and coworkers [9,10].

In our study we want to investigate whether for some values of the six kinetic parameters ($k_1[A]$, $k_2[B]$, k_{-1}, k_{-2}, k_3^0 , μ) sustained oscillations can exist.

IId] Steady state equations

At steady state, equations (8) and (9) become:

$$0=k_1[A](1-x_s-y_s)-k_{-1}x_s-k_3^0 e^{-\mu y_s}x_s y_s \qquad (10)$$

$$0=k_2[B](1-x_s-y_s)-k_{-2}y_s-k_3^0 e^{-\mu y_s}x_s y_s \qquad (11)$$

where x_s and y_s denote the steady state values of x and y, respectively.

combining (10) and (11) we obtain

$$y_s = \beta_1 x_s + \beta_2 \qquad (12)$$

where

$$\beta_1 = \frac{\{K_{-1} + K_1[A] - K_2[B]\}}{\{K_{-2} - K_1[A] + K_2[B]\}}, \beta_2 = \frac{\{K_2[B] - K_1[A]\}}{\{K_{-2} - K_1[A] + K_2[B]\}} \qquad (12a)$$

Assuming that $\beta_1 \neq 0$, which implies $k_{-1} + k_1 [A] \neq k_2[B]$,

(12) gives

$$X_s = \frac{1}{\beta_1}(y_s - \beta_2) \qquad (13)$$

substituting (13) in (10) and further assuming that

$y_s(y_s - \beta_2) \neq 0$, we obtain

$$e^{-\mu y_s} = \frac{\beta_1 K_1[A](1-\beta_2) + \beta_2[K_{-1} + K_1[A](1+\beta_1)]}{K_3^\circ y_s(y_s - \beta_2)} - \frac{[K_{-1} + K_1[A](1+\beta_1)]}{K_3^\circ(y_s - \beta_2)} \qquad (14)$$

CHAPTER III

Here we linearize equations (8) and (9) about the steady state and use the first method of Liapunov to determine the local stability of the critical points. Next, we derive expressions for the determinant and trace of $\underline{A}$ in the special case $k_1[A] = k_2[B]$. Our purpose is to demonstrate that when $\beta_2 = 0$ it is easier to classify the critical points of the linearized system (27) by determining the sign of det$\underline{A}$ and tr$\underline{A}$, than when $\beta_2 \neq 0$.

IIIa] Linerization of the dynamic equations.

The net rates of adsorption of reactants A(g) and B(g) on the catalytic surface are given by the ordinary differential equations:

$$\frac{dx}{dt} = K_1[A](1-x-y) - K_{-1}x - K_3^{\circ} e^{-\mu y} xy \equiv f_1(x,y) \qquad (8)$$

$$\frac{dy}{dt} = K_2[B](1-x-y) - K_{-2}y - K_3^{\circ} e^{-\mu y} xy \equiv f_2(x,y) \qquad (9)$$

Our purpose is to investigate whether for some values of the six kinetic parameters sustained oscillations can exist. In other words, we want to find kinetic parameters for which equations (8) and (9) give rise to limit cycles.

The first method of Liapunov consists of examining the properties of equations (8) and (9) linearized about the steady state. Linearization of (8) and (9) yields

$$\frac{d\underline{Y}}{dt} = \underline{A}\,\underline{Y}$$

where

$$\underline{Y} = \begin{bmatrix} x - x_s \\ y - y_s \end{bmatrix}, \quad \underline{A} = \begin{bmatrix} \frac{\partial f_1}{\partial x} & \frac{\partial f_1}{\partial y} \\ \frac{\partial f_2}{\partial x} & \frac{\partial f_2}{\partial y} \end{bmatrix}_{\substack{x = x_s \\ y = y_s}}$$

where

$$\frac{\partial f_1}{\partial x} = -K_1[A] - K_{-1} - K_3^{\circ} y\, e^{-\mu y}, \quad \frac{\partial f_1}{\partial y} = -K_1[A] + K_3^{\circ} x\, e^{-\mu y}(\mu y - 1)$$

$$\frac{\partial f_2}{\partial x} = -K_2[B] - K_3^{\circ} y\, e^{-\mu y}, \quad \frac{\partial f_2}{\partial y} = -K_2[B] - K_{-2} + K_3^{\circ} x\, e^{-\mu y}(\mu y - 1)$$

The local stability character of the steady states is determined by the sign of the real part of the eigenvalues of $\underline{A}$. These eigenvalues, λ_1, λ_2, are the roots of the characteristic equation

$$\lambda^2 - (\mathrm{tr}\underline{A})\lambda + (\det\underline{A}) = 0$$

where the determinant of $\underline{A}$

$$\det\underline{A} = \left[\frac{\partial f_1}{\partial x}\frac{\partial f_2}{\partial y} - \frac{\partial f_2}{\partial x}\frac{\partial f_1}{\partial y}\right]_{\substack{x = x_s \\ y = y_s}}$$

and the trace of $\underline{A}$

$$\mathrm{tr}\underline{A} = \left[\frac{\partial f_1}{\partial x} + \frac{\partial f_2}{\partial y}\right]_{\substack{x = x_s \\ y = y_s}}$$

Algebraic substitution yields

$$\det\underline{A} = \alpha_1 + e^{-\mu y_s}\left[\alpha_2 y_s + \alpha_3 x_s(\mu y_s - 1)\right] \tag{15}$$

$$\mathrm{tr}\underline{A} = -\beta + K_3^{\circ} e^{-\mu y_s}\left[x_s(\mu y_s - 1) - y_s\right] \tag{16}$$

where

$$\alpha_1 \equiv \left\{K_{-1}K_2[B] + K_{-2}K_1[A] + K_{-1}K_{-2}\right\} \tag{17}$$

$$\alpha_2 \equiv K_3^\circ \{K_2[B] - K_1[A] + K_{-2}\} \qquad (18)$$

$$\alpha_3 \equiv K_3^\circ \{K_2[B] - K_1[A] - K_{-1}\} \qquad (19)$$

$$\beta \equiv \{K_1[A] + K_{-1} + K_2[B] + K_{-2}\} \qquad (20)$$

We can eliminate x_s from (15) and (16) by using the relation(13),

$$x_s = (y_s - \beta_2)/\beta_1$$

to obtain

$$\det \underline{A} = \alpha_1 + e^{-\mu y_s}\left\{\alpha_2 y_s + \alpha_3\left(\frac{y_s-\beta_2}{\beta_1}\right)(\mu y_s - 1)\right\} \qquad (21)$$

$$\mathrm{tr}\,\underline{A} = -\beta + K_3^\circ e^{-\mu y_s}\left\{(\mu y_s - 1)\left(\frac{y_s-\beta_2}{\beta_1}\right) - y_s\right\} \qquad (22)$$

We can eliminate the exponential term in (21) and (22) by using (14) :

$$e^{-\mu y_s} = \frac{\beta_1 K_1[A](1-\beta_2) + \beta_2[K_{-1} + K_1[A](1+\beta_1)]}{K_3^\circ y_s(y_s-\beta_2)} - \frac{[K_{-1}+K_1[A](1+\beta_1)]}{K_3^\circ(y_s-\beta_2)}$$

to obtain

$$\det \underline{A} = \alpha_1 + \frac{\alpha_2(\mathcal{H} - \Theta y_s)}{K_3^\circ(y_s-\beta_2)} + \frac{\alpha_3(\mu y_s - 1)(\mathcal{H} - \Theta y_s)}{K_3^\circ \beta_1 y_s} \qquad (23)$$

$$\mathrm{tr}\,\underline{A} = -\beta - \frac{(\mathcal{H} - \Theta y_s)}{(y_s-\beta_2)} + \frac{(\mu y_s - 1)(\mathcal{H} - \Theta y_s)}{\beta_1 y_s} \qquad (24)$$

where

$$\mathcal{H} \equiv K_1[A](\beta_1+\beta_2) + K_{-1}\beta_2 = \frac{K_{-1}K_2[B]}{K_{-2} + K_2[B] - K_1[A]} \qquad (25)$$

$$\Theta \equiv [K_{-1} + K_1[A](1+\beta_1)] = \frac{K_{-1}K_{-2} + K_{-1}K_2[B] + K_{-2}K_1[A]}{K_{-2} + K_2[B] - K_1[A]} \qquad (26)$$

IIIb] <u>Classification of the critical points of the linearized system.</u>

We found that the linearized equations are given by

$$d\underline{Y}/dt = \underline{A}\ \underline{Y} \qquad (27)$$

and the determinant and trace of $\underline{A}$ are given by (23) and (24), respectively. We now state the following theorem[9]:

Theorem 3.1. Let $D = (\mathrm{tr}\underline{A})^2 - 4(\det\underline{A})$. Then, the critical points of the linearized system (27) are classified as follows:

1. If $\det\underline{A} < 0$, then the critical point is a saddle point.
2. Let $\det\underline{A} > 0$. Then

(i) The steady state is an unstable focus if $\mathrm{tr}\underline{A} > 0$ and $D < 0$, and an unstable node if $\mathrm{tr}\underline{A} > 0$ and $D > 0$.

(ii) The steady state is a stable focus if $\mathrm{tr}\underline{A} < 0$ and $D < 0$, and a stable node if $\mathrm{tr}\underline{A} < 0$ and $D > 0$.

(iii) The steady state is a center if $\mathrm{tr}\underline{A} = 0$.

(iv) The steady state is a stable or unstable node if $D=0$.

3. Let $\det\underline{A} = 0$. The critical point is degenerate in the sense that the phase plane consists entirely of critical points or entirely of parallel straight lines and critical points.

The type of critical point for the nonlinear equations (8) and (9) is the same as that for the linear problem in cases 1 and 2 above except in the case of the center. The critical point is either a center or a spiral for the nonlinear problem.

Remark 1: For some combination of the six kinetic parameters ($k_1[A]$, $k_2[B]$, k_{-1}, k_{-2}, k_3^0, μ) each of the cases in (1)-(3) actually occurs for the nonlinear system.

Remark 2: The critical points are roots of equation (14) in the interval (0,1).

IIIc] The special case $k_1[A] = k_2[B]$

Suppose that $k_1[A] = k_2[B]$. Then (12a) become

$$\beta_1 = k_{-1}/k_{-2} \tag{28}$$

$$\beta_2 = 0 \tag{29}$$

Equations (17)-(20) become

$$\alpha_1 \equiv \{k_1[A](k_{-1}+k_{-2}) + k_{-1}k_{-2}\} \tag{30}$$

$$\alpha_2 \equiv k_3^0 k_{-2} \tag{31}$$

$$\alpha_3 \equiv -k_3^0 k_{-1} \tag{32}$$

$$\beta \equiv \{2k_1[A] + k_{-1} + k_{-2}\} \tag{33}$$

Equations (25)-(26) become

$$\mathcal{H} \equiv k_1[A]k_{-1}/k_{-2} \tag{34}$$

$$\Theta \equiv \left[k_{-1} + k_1[A]\left(1 + \frac{k_{-1}}{k_{-2}}\right)\right] \tag{35}$$

Since $\beta_2 = 0$, (23) and (24) become

$$\det \underline{A} = \alpha_1 + \frac{(\mathcal{H} - \Theta y_s)[\alpha_2\beta_1 + \alpha_3(\mu y_s - 1)]}{k_3^0\,\beta_1\,y_s} \tag{36}$$

$$\operatorname{tr}\underline{A} = -\beta + \frac{(\mathcal{H} - \Theta y_s)[(\mu y_s - 1) - \beta_1]}{\beta_1 y_s} \tag{37}$$

Since $\beta_1 > 0$, $\alpha_3 < 0$, and $0 < y_s < 1$, it follows that

$\operatorname{sgn}(\det\underline{A}) = \operatorname{sgn}(\Phi(y_s))$ and $\operatorname{sgn}(\operatorname{tr}\underline{A}) = \operatorname{sgn}(G(y_s))$

where

$$\Phi(y_s) \equiv \left[-K_3^{\circ}\beta_1 y_s/\alpha_3\right](\det\underline{A}) \tag{38}$$

$$G(y_s) \equiv (\beta_1 y_s)(\mathrm{tr}\underline{A}) \tag{39}$$

Substituting (28)-(35) in (36)-(37) and then in (38)-(39), we obtain that

$$\Phi(y_s) = \gamma y_s^2 - \varepsilon y_s + \vartheta \tag{40}$$

$$G(y_s) = -\gamma y_s^2 + \varepsilon' y_s - \vartheta' \tag{41}$$

where

$$\gamma \equiv \mu\left[K_{-1} + K_1[A]\left(1 + \frac{K_{-1}}{K_{-2}}\right)\right] \tag{42}$$

$$\varepsilon \equiv \left[K_{-1} + K_1[A]\left(1 + \frac{K_{-1}}{K_{-2}}\right) + \mu K_1[A]\frac{K_{-1}}{K_{-2}}\right] \tag{43}$$

$$\vartheta \equiv \left[2K_1[A]\frac{K_{-1}}{K_{-2}}\right] \tag{44}$$

$$\varepsilon' \equiv \left[\mu K_1[A]\frac{K_{-1}}{K_{-2}} + K_1[A]\left(1 + \left(\frac{K_{-1}}{K_{-2}}\right)^2\right)\right] \tag{45}$$

$$\vartheta' \equiv \frac{K_1[A]K_{-1}}{K_{-2}}\left(1 + \frac{K_{-1}}{K_{-2}}\right) \tag{46}$$

Note that when $k_1[A] = k_2[B]$, $\beta_2 = 0$, equation (14) becomes

$$K_3^{\circ} y_s^2 e^{-\mu y_s} + \left\{K_{-1} + K_1[A]\left(1 + \frac{K_{-1}}{K_{-2}}\right)\right\} y_s - K_1[A]\left(\frac{K_{-1}}{K_{-2}}\right) = 0 \tag{47}$$

and the critical points are roots of (47), where $0 < y_s < 1$.

Remark 3: Undoubtedly, theorem 3.1 also applies in the special case $k_1[A] = k_2[B]$, where instead of examining the sign of $\det\underline{A}$ and $\mathrm{tr}\underline{A}$ we are interested in the sign of the polynomials $\Phi(y_s)$ and $G(y_s)$ which are given by (40)-(41).

IIId] Roots of the polynomials (40)-(41).

Consider the equations

$$\Phi(\xi)=\gamma\xi^2-\varepsilon\xi+\vartheta=0 \tag{48}$$

$$\mathfrak{G}(\omega)=-\gamma\omega^2+\varepsilon'\omega-\vartheta'=0 \tag{49}$$

Let Δ_ϕ and $\Delta_{\mathfrak{G}}$ denote the discriminants of the equations (48) and (49), respectively. Then

$$\Delta_\phi=\varepsilon^2-4\gamma\vartheta \tag{50}$$

$$\Delta_{\mathfrak{G}}=\varepsilon'^2-4\gamma\vartheta' \tag{51}$$

Suppose now that

$$\Phi(\rho_1)=\Phi(\rho_2)=0$$

and $\mathfrak{G}(\Psi_1)=\mathfrak{G}(\Psi_2)=0$

Then

$$\rho_1=\frac{\varepsilon+\sqrt{\varepsilon^2-4\gamma\vartheta}}{2\gamma},\ \rho_2=\frac{\varepsilon-\sqrt{\varepsilon^2-4\gamma\vartheta}}{2\gamma} \tag{52}$$

and

$$\Psi_1=\frac{\varepsilon'+\sqrt{\varepsilon'^2-4\gamma\vartheta'}}{2\gamma},\ \Psi_2=\frac{\varepsilon'-\sqrt{\varepsilon'^2-4\gamma\vartheta'}}{2\gamma} \tag{53}$$

Remark 4: When $\varepsilon^2-4\gamma\vartheta=0$, then $\rho_1=\rho_2=\rho=\frac{\varepsilon}{2\gamma}$ (54)

When $\varepsilon'^2-4\gamma\vartheta'=0$, then $\Psi_1=\Psi_2=\Psi=\varepsilon'/2\gamma$ (55)

Remark 5: ρ_1, ρ_2 are also roots of the equ. $\det\underline{A}=0$.

Ψ_1, Ψ_2 are also roots of the equ. $\mathrm{tr}\underline{A}=0$.

CHAPTER IV

Here we describe a procedure which helps in classifying the critical points of the linearized system (27) for the special case $k_1[A] = k_2[B]$. We emphasize the importance of the nature and relative positions of ρ_1, ρ_2, Ψ_1, Ψ_2, and derive necessary and sufficient conditions for all possible arrangements for the root positions for the polynomials $\Phi(y_s)$ and $G(y_s)$.

IVa] The nature of the roots of $\det\underline{A} = 0$ and $\mathrm{tr}\underline{A} = 0$.

In the previous chapter we derived expressions for $\det\underline{A}$ and $\mathrm{tr}\underline{A}$ for the special case $k_1[A] = k_2[B]$. We also obtained the polynomials

$$\phi(y_s) = \gamma y_s^2 - \varepsilon y_s + \vartheta \tag{40}$$

$$G(y_s) = -\gamma y_s^2 + \varepsilon' y_s - \vartheta' \tag{41}$$

which have the same sign as $\det\underline{A}$ and $\mathrm{tr}\underline{A}$, respectively. These polynomials are very helpful in classifying the critical points of the linearized system (27) for various values of the kinetic parameters, by using theorem 3.1.

The roots ρ_1, ρ_2 of

$$\phi(\xi) = \gamma\xi^2 - \varepsilon\xi + \vartheta = 0$$

are given by (52), while the roots Ψ_1, Ψ_2 of

$$G(\omega) = -\gamma\xi^2 + \varepsilon'\xi - \vartheta' = 0$$

are given by (53). Note that ρ_1, ρ_2 are roots of $\det\underline{A}$ and Ψ_1,

Ψ_2 are roots of tr$\underline{A}$.

The following cases can be distinguished with respect to the nature of the roots ρ_1, ρ_2, Ψ_1, Ψ_2:

(A) The roots of $\Phi(\xi) = 0$ and $G(\omega) = 0$ are all real and unequal; that is, $\rho_1 > \rho_2$ and $\Psi_1 > \Psi_2$ and the two equations have no common roots.

(B) ρ_1, ρ_2, Ψ_1, Ψ_2 are real. However, the roots of either $\Phi(\xi) = 0$ or $G(\omega) = 0$ are equal; that is, $\rho_1 = \rho_2 = \rho$ and $\Psi_1 > \Psi_2$, or $\Psi_1 = \Psi_2 = \Psi$ and $\rho_1 > \rho_2$. There is also the trivial case $\rho_1 = \rho_2 = \Psi_1 = \Psi_2$.

(C) The roots of either $\Phi(\xi) = 0$, or $G(\omega) = 0$, or of both of them are complex. Here, we can distinguish the following subcases:

(i) ρ_1, ρ_2 are complex and $\Psi_1 > \Psi_2$.

(ii) ρ_1, ρ_2 are complex and $\Psi_1 = \Psi_2 = \Psi$.

(iii) Ψ_1, Ψ_2 are complex and $\rho_1 > \rho_2$.

(iv) Ψ_1, Ψ_2 are complex and $\rho_1 = \rho_2 = \rho$.

(v) ρ_1, ρ_2, Ψ_1, Ψ_2 are complex.

IVb] Relative positions of ρ_1, ρ_2, Ψ_1, Ψ_2.

According to theorem 3.1, we need to know the sign of $\Phi(y_s)$ and $G(y_s)$ in order to classify the critical points of the linearized system (27). The sign of $\Phi(y_s)$ and $G(y_s)$ depends, in turn, on the position of $y_s \in (0,1)$ with respect to the roots of $\Phi(\xi) = 0$ and $G(\omega) = 0$.

However, before examining the position of $y_s \in (0,1)$ with respect to ρ_1, ρ_2, Ψ_1, Ψ_2, it should be emphasized that for the cases (A)-(C) a large number of possible arrangements for the root positions exists, and that it is relatively easy to derive the necessary and sufficient conditions for each of them.

The necessary and sufficient conditions for all possible arrangements for the root positions for cases (A)-(C) are presented next. The detailed derivation of these conditions is shown in the Appendix.

CASE A

a1] $0 < \rho_2 < \Psi_2 < \rho_1 < \Psi_1 < 1$

$$\gamma(\vartheta'-\vartheta)^2 < (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$2\gamma > \varepsilon' > \varepsilon$$
$$(\gamma-\varepsilon'+\vartheta') > 0$$

a2] $0 < \rho_2 < \Psi_2 < \rho_1 < 1 < \Psi_1$

$$\gamma(\vartheta'-\vartheta)^2 < (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon < \inf(\varepsilon', 2\gamma)$$
$$(\varepsilon-\vartheta) < \gamma < (\varepsilon'-\vartheta')$$

a3] $0 < \rho_2 < \Psi_2 < 1 < \rho_1 < \Psi_1$

$$\gamma(\vartheta'-\vartheta)^2 < (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon' > \varepsilon$$
$$\gamma < \inf\left[(\varepsilon'-\vartheta'), (\varepsilon-\vartheta)\right]$$

a4] $0 < \rho_2 < 1 < \Psi_2 < \rho_1 < \Psi_1$

$$\gamma(\vartheta'-\vartheta)^2 < (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon' > \sup(\varepsilon, 2\gamma)$$
$$(\varepsilon'-\vartheta') < \gamma < (\varepsilon-\vartheta)$$

a5] $1 < \rho_2 < \Psi_2 < \rho_1 < \Psi_1$

$$\gamma(\vartheta'-\vartheta)^2 < (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$2\gamma < \varepsilon < \varepsilon'$$
$$(\gamma-\varepsilon+\vartheta) > 0$$

b1] $0 < \Psi_2 < \rho_2 < \Psi_1 < \rho_1 < 1$

$$\gamma(\vartheta'-\vartheta)^2 < (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon' < \varepsilon < 2\gamma$$
$$(\gamma-\varepsilon+\vartheta) > 0$$

b2] $0 < \Psi_2 < \rho_2 < \Psi_1 < 1 < \rho_1$

$$\gamma(\vartheta'-\vartheta)^2 < (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon' < \inf(\varepsilon, 2\gamma)$$
$$(\varepsilon'-\vartheta') < \gamma < (\varepsilon-\vartheta)$$

b3] $0 < \Psi_2 < \rho_2 < 1 < \Psi_1 < \rho_1$

$$\gamma(\vartheta'-\vartheta)^2 < (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon' < \varepsilon$$
$$\gamma < \inf\{(\varepsilon-\vartheta), (\varepsilon'-\vartheta')\}$$

b4] $0 < \Psi_2 < 1 < \rho_2 < \Psi_1 < \rho_1$

$$\gamma(\vartheta'-\vartheta)^2 < (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon > \sup(\varepsilon', 2\gamma)$$
$$(\varepsilon-\vartheta) < \gamma < (\varepsilon'-\vartheta')$$

b5] $1 < \Psi_2 < \rho_2 < \Psi_1 < \rho_1$

$$\gamma(\vartheta'-\vartheta)^2 < (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$2\gamma < \varepsilon' < \varepsilon$$
$$(\gamma-\varepsilon'+\vartheta') > 0$$

c1] $0 < \rho_2 < \Psi_2 < \Psi_1 < \rho_1 < 1$

$$\varepsilon'^2 - 4\gamma\vartheta' > 0$$
$$\gamma(\vartheta'-\vartheta)^2 > (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon'(\varepsilon'-\varepsilon) < 2\gamma(\vartheta'-\vartheta)$$
$$\gamma > \sup\left\{ \frac{\varepsilon}{2}, (\varepsilon-\vartheta)\right\}$$

c2] $0 < \rho_2 < \Psi_2 < \Psi_1 < 1 < \rho_1$

$$\varepsilon'^2 - 4\gamma\vartheta' > 0$$
$$\gamma(\vartheta'-\vartheta)^2 > (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon'(\varepsilon'-\varepsilon) < 2\gamma(\vartheta'-\vartheta)$$
$$\varepsilon' < 2\gamma$$
$$(\varepsilon'-\vartheta') < \gamma < (\varepsilon-\vartheta)$$

c3] $0 < \rho_2 < \Psi_2 < 1 < \Psi_1 < \rho_1$

$$\varepsilon'^2 - 4\gamma\vartheta' > 0$$
$$\gamma(\vartheta'-\vartheta)^2 > (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon'(\varepsilon'-\varepsilon) < 2\gamma(\vartheta'-\vartheta)$$
$$(\gamma-\varepsilon'+\vartheta') < 0$$

c4] $0 < \rho_2 < 1 < \Psi_2 < \Psi_1 < \rho_1$

$$\varepsilon'^2 - 4\gamma\vartheta' > 0$$
$$\gamma(\vartheta'-\vartheta)^2 > (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon'(\varepsilon'-\varepsilon) < 2\gamma(\vartheta'-\vartheta)$$
$$(\varepsilon'-\vartheta) < \gamma < (\varepsilon-\vartheta)$$
$$\varepsilon' > 2\gamma$$

c5] $1 < \rho_2 < \psi_2 < \psi_1 < \rho_1$

$$\varepsilon'^2 - 4\gamma\vartheta' > 0$$
$$\gamma(\vartheta' - \vartheta)^2 > (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta')$$
$$\varepsilon'(\varepsilon' - \varepsilon) < 2\gamma(\vartheta' - \vartheta)$$
$$(\varepsilon - \vartheta) < \gamma < \frac{\varepsilon}{2}$$

d1] $0 < \psi_2 < \rho_2 < \rho_1 < \psi_1 < 1$

$$\varepsilon^2 - 4\gamma\vartheta > 0$$
$$\gamma(\vartheta' - \vartheta)^2 > (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta')$$
$$\varepsilon(\varepsilon' - \varepsilon) > 2\gamma(\vartheta' - \vartheta)$$
$$\gamma > \sup\left\{\frac{\varepsilon'}{2}, (\varepsilon' - \vartheta')\right\}$$

d2] $0 < \psi_2 < \rho_2 < \rho_1 < 1 < \psi_1$

$$\varepsilon^2 - 4\gamma\vartheta > 0$$
$$\gamma(\vartheta' - \vartheta)^2 > (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta')$$
$$\varepsilon(\varepsilon' - \varepsilon) > 2\gamma(\vartheta' - \vartheta)$$
$$\sup\left\{\frac{\varepsilon}{2}, (\varepsilon - \vartheta)\right\} < \gamma < (\varepsilon' - \vartheta')$$

d3] $0 < \psi_2 < \rho_2 < 1 < \rho_1 < \psi_1$

$$\varepsilon^2 - 4\gamma\vartheta > 0$$
$$\gamma(\vartheta' - \vartheta)^2 > (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta')$$
$$\varepsilon(\varepsilon' - \varepsilon) > 2\gamma(\vartheta' - \vartheta)$$
$$(\gamma - \varepsilon + \vartheta) < 0$$

d4] $0 < \psi_2 < 1 < \rho_2 < \rho_1 < \psi_1$

$$\varepsilon^2 - 4\gamma\vartheta > 0$$
$$\gamma(\vartheta' - \vartheta) > (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta')$$
$$\varepsilon(\varepsilon' - \varepsilon) > 2\gamma(\vartheta' - \vartheta)$$
$$(\varepsilon - \vartheta) < \gamma < \inf\left\{\frac{\varepsilon}{2}, (\varepsilon' - \vartheta')\right\}$$

d5] $1<\psi_2<\rho_2<\rho_1<\psi_1$

$$\varepsilon^2-4\gamma\vartheta>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon(\varepsilon'-\varepsilon)>2\gamma(\vartheta'-\vartheta)$$
$$(\varepsilon'-\vartheta')<\gamma<\frac{\varepsilon'}{2}$$

e1] $0<\rho_2<\rho_1<\psi_2<\psi_1<1$

$$\varepsilon^2-4\gamma\vartheta>0$$
$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon(\varepsilon'-\varepsilon)<2\gamma(\vartheta'-\vartheta)<\varepsilon'(\varepsilon'-\varepsilon)$$
$$\varepsilon<\varepsilon'<2\gamma$$
$$(\gamma-\varepsilon'+\vartheta')>0$$

e2] $0<\rho_2<\rho_1<\psi_2<1<\psi_1$

$$\varepsilon^2-4\gamma\vartheta>0$$
$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon(\varepsilon'-\varepsilon)<2\gamma(\vartheta'-\vartheta)<\varepsilon'(\varepsilon'-\varepsilon)$$
$$\varepsilon'>\varepsilon$$
$$(\gamma-\varepsilon'+\vartheta')<0$$

e3] $0<\rho_2<\rho_1<1<\psi_2<\psi_1$

$$\varepsilon^2-4\gamma\vartheta>0$$
$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon(\varepsilon'-\varepsilon)<2\gamma(\vartheta'-\vartheta)<\varepsilon'(\varepsilon'-\varepsilon)$$
$$\sup\left\{\frac{\varepsilon}{2},(\varepsilon'-\vartheta'),(\varepsilon-\vartheta)\right\}<\gamma<\frac{\varepsilon'}{2}$$

e4] $0<\rho_2<1<\rho_1<\psi_2<\psi_1$

$$\varepsilon^2-4\gamma\vartheta>0$$
$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon(\varepsilon'-\varepsilon)<2\gamma(\vartheta'-\vartheta)<\varepsilon'(\varepsilon'-\varepsilon)$$
$$\varepsilon'>\varepsilon$$
$$(\gamma-\varepsilon+\vartheta)<0$$

e5] $1<\rho_2<\rho_1<\psi_2<\psi_1$

$$\varepsilon^2-4\gamma\vartheta>0$$
$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon(\varepsilon'-\varepsilon)<2\gamma(\vartheta'-\vartheta)<\varepsilon'(\varepsilon'-\varepsilon)$$
$$2\gamma<\varepsilon<\varepsilon'$$
$$(\gamma-\varepsilon+\vartheta)>0$$

f1] $0<\psi_2<\psi_1<\rho_2<\rho_1<1$

$$\varepsilon^2-4\gamma\vartheta>0$$
$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon(\varepsilon'-\varepsilon)<2\gamma(\vartheta'-\vartheta)<\varepsilon'(\varepsilon'-\varepsilon)$$
$$\varepsilon'<\varepsilon<2\gamma$$
$$(\gamma-\varepsilon+\vartheta)>0 .$$

f2] $0<\psi_2<\psi_1<\rho_2<1<\rho_1$

$$\varepsilon^2-4\gamma\vartheta>0$$
$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon(\varepsilon'-\varepsilon)<2\gamma(\vartheta'-\vartheta)<\varepsilon'(\varepsilon'-\varepsilon)$$
$$\varepsilon'<\varepsilon$$
$$(\gamma-\varepsilon+\vartheta)<0$$

f3] $0<\psi_2<\psi_1<1<\rho_2<\rho_1$

$$\varepsilon^2-4\gamma\vartheta>0$$
$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon(\varepsilon'-\varepsilon)<2\gamma(\vartheta'-\vartheta)<\varepsilon'(\varepsilon'-\varepsilon)$$
$$\sup\left\{\frac{\varepsilon'}{2},(\varepsilon-\vartheta),(\varepsilon'-\vartheta')\right\}<\gamma<\frac{\varepsilon}{2}$$

f4] $0<\psi_2<1<\psi_1<\rho_2<\rho_1$

$$\varepsilon^2-4\gamma\vartheta>0$$
$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon(\varepsilon'-\varepsilon)<2\gamma(\vartheta'-\vartheta)<\varepsilon'(\varepsilon'-\varepsilon)$$
$$\varepsilon'<\varepsilon$$
$$(\gamma-\varepsilon'+\vartheta')<0$$

f5] $1<\psi_2<\psi_1<\rho_2<\rho_1$

$$\varepsilon^2-4\gamma\vartheta>0$$
$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon(\varepsilon'-\varepsilon)<2\gamma(\vartheta'-\vartheta)<\varepsilon'(\varepsilon'-\varepsilon)$$
$$2\gamma<\varepsilon'<\varepsilon$$
$$(\gamma-\varepsilon'+\vartheta')>0$$

CASE B

a1] $0<\rho<\Psi_2<\Psi_1<1$

$$\varepsilon^2=4\gamma\vartheta$$
$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$2\gamma\vartheta'>\varepsilon\left(\varepsilon'-\frac{\varepsilon}{2}\right)$$
$$\varepsilon<\varepsilon'<2\gamma$$
$$(\gamma-\varepsilon'+\vartheta')>0$$

a2] $0<\rho<\Psi_2<1<\Psi_1$

$$\varepsilon^2=4\gamma\vartheta$$
$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$2\gamma\vartheta'>\varepsilon\left(\varepsilon'-\frac{\varepsilon}{2}\right)$$
$$\varepsilon'>\varepsilon$$
$$(\gamma-\varepsilon'+\vartheta')<0$$

a3] $0<\rho<1<\Psi_2<\Psi_1$

$$\varepsilon^2=4\gamma\vartheta$$
$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$2\gamma\vartheta'>\varepsilon\left(\varepsilon'-\frac{\varepsilon}{2}\right)$$
$$\sup\left\{\frac{\varepsilon}{2},(\varepsilon'-\vartheta')\right\}<\gamma<\frac{\varepsilon'}{2}$$

a4] $1<\rho<\Psi_2<\Psi_1$

$$\varepsilon^2=4\gamma\vartheta$$
$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$2\gamma\vartheta'>\varepsilon\left(\varepsilon'-\frac{\varepsilon}{2}\right)$$
$$2\gamma<\varepsilon<\varepsilon'$$

b1] $0 < \Psi_2 < \Psi_1 < \rho < 1$

$$\varepsilon^2 = 4\gamma\vartheta$$
$$\varepsilon'^2 - 4\gamma\vartheta' > 0$$
$$2\gamma\vartheta' > \varepsilon\left(\varepsilon' - \frac{\varepsilon}{2}\right)$$
$$\varepsilon' < \varepsilon < 2\gamma$$

b2] $0 < \Psi_2 < \Psi_1 < 1 < \rho$

$$\varepsilon^2 = 4\gamma\vartheta$$
$$\varepsilon'^2 - 4\gamma\vartheta' > 0$$
$$2\gamma\vartheta' > \varepsilon\left(\varepsilon' - \frac{\varepsilon}{2}\right)$$
$$\sup\left\{\frac{\varepsilon'}{2}, (\varepsilon' - \vartheta')\right\} < \gamma < \frac{\varepsilon}{2}$$

b3] $0 < \Psi_2 < 1 < \Psi_1 < \rho$

$$\varepsilon^2 = 4\gamma\vartheta$$
$$\varepsilon'^2 - 4\gamma\vartheta' > 0$$
$$2\gamma\vartheta' > \varepsilon\left(\varepsilon' - \frac{\varepsilon}{2}\right)$$
$$(\gamma - \varepsilon' + \vartheta') < 0$$
$$\varepsilon > \varepsilon'$$

b4] $1 < \Psi_2 < \Psi_1 < \rho$

$$\varepsilon^2 = 4\gamma\vartheta$$
$$\varepsilon'^2 - 4\gamma\vartheta' > 0$$
$$2\gamma\vartheta' > \varepsilon\left(\varepsilon' - \frac{\varepsilon}{2}\right)$$
$$2\gamma < \varepsilon' < \varepsilon$$
$$(\gamma - \varepsilon' + \vartheta') > 0$$

c1] $0 < \Psi_2 < \rho < \Psi_1 < 1$

$$\varepsilon^2 = 4\gamma\vartheta$$
$$2\gamma\vartheta' < \varepsilon\left(\varepsilon' - \frac{\varepsilon}{2}\right)$$
$$\gamma > \sup\left\{\frac{\varepsilon'}{2}, (\varepsilon' - \vartheta')\right\}$$

c2] $0 < \Psi_2 < \rho < 1 < \Psi_1$

$$\varepsilon^2 = 4\gamma\vartheta$$
$$2\gamma\vartheta' < \varepsilon\left(\varepsilon' - \frac{\varepsilon}{2}\right)$$
$$\frac{\varepsilon}{2} < \gamma < (\varepsilon' - \vartheta')$$

c3] $0 < \Psi_2 < 1 < \rho < \Psi_1$

$$\varepsilon^2 = 4\gamma\vartheta$$
$$2\gamma\vartheta' < \varepsilon\left(\varepsilon' - \frac{\varepsilon}{2}\right)$$
$$\gamma < \inf\left\{(\varepsilon' - \vartheta'),\ \frac{\varepsilon}{2}\right\}$$

c4] $1 < \Psi_2 < \rho < \Psi_1$

$$\varepsilon^2 = 4\gamma\vartheta$$
$$2\gamma\vartheta' < \varepsilon\left(\varepsilon' - \frac{\varepsilon}{2}\right)$$
$$(\varepsilon' - \vartheta') < \gamma < \frac{\varepsilon'}{2}$$

d1] $0 < \Psi < \rho_2 < \rho_1 < 1$

$$\varepsilon'^2 = 4\gamma\vartheta'$$
$$\varepsilon^2 - 4\gamma\vartheta > 0$$
$$2\gamma\vartheta > \varepsilon'\left(\varepsilon - \frac{\varepsilon'}{2}\right)$$
$$\varepsilon' < \varepsilon < 2\gamma$$
$$(\gamma - \varepsilon + \vartheta) > 0$$

d2] $0 < \Psi < \rho_2 < 1 < \rho_1$

$$\varepsilon'^2 = 4\gamma\vartheta'$$
$$\varepsilon^2 - 4\gamma\vartheta > 0$$
$$2\gamma\vartheta > \varepsilon'\left(\varepsilon - \frac{\varepsilon'}{2}\right)$$
$$\varepsilon > \varepsilon'$$
$$(\gamma - \varepsilon + \vartheta) < 0$$

d3] $0 < \Psi < 1 < \rho_2 < \rho_1$

$$\varepsilon'^2 = 4\gamma\vartheta'$$
$$\varepsilon^2 - 4\gamma\vartheta > 0$$
$$2\gamma\vartheta > \varepsilon'\left(\varepsilon - \frac{\varepsilon'}{2}\right)$$
$$\sup\left\{\frac{\varepsilon'}{2},\ (\varepsilon - \vartheta)\right\} < \gamma < \frac{\varepsilon}{2}$$

d4] $1 < \psi < \rho_2 < \rho_1$

$$\varepsilon'^2 = 4\gamma\vartheta'$$
$$\varepsilon^2 - 4\gamma\vartheta > 0$$
$$2\gamma\vartheta > \varepsilon'\left(\varepsilon - \frac{\varepsilon'}{2}\right)$$
$$2\gamma < \varepsilon' < \varepsilon$$

e1] $0 < \rho_2 < \rho_1 < \psi < 1$

$$\varepsilon'^2 = 4\gamma\vartheta'$$
$$\varepsilon^2 - 4\gamma\vartheta > 0$$
$$2\gamma\vartheta > \varepsilon'\left(\varepsilon - \frac{\varepsilon'}{2}\right)$$
$$\varepsilon < \varepsilon' < 2\gamma$$

e2] $0 < \rho_2 < \rho_1 < 1 < \psi$

$$\varepsilon'^2 = 4\gamma\vartheta'$$
$$\varepsilon^2 - 4\gamma\vartheta > 0$$
$$2\gamma\vartheta > \varepsilon'\left(\varepsilon - \frac{\varepsilon'}{2}\right)$$
$$\sup\left\{(\varepsilon - \vartheta), \frac{\varepsilon}{2}\right\} < \gamma < \frac{\varepsilon'}{2}$$

e3] $0 < \rho_2 < 1 < \rho_1 < \psi$

$$\varepsilon'^2 = 4\gamma\vartheta'$$
$$\varepsilon^2 - 4\gamma\vartheta > 0$$
$$2\gamma\vartheta > \varepsilon'\left(\varepsilon - \frac{\varepsilon'}{2}\right)$$
$$\varepsilon' > \varepsilon$$
$$(\gamma - \varepsilon + \vartheta) < 0$$

e4] $1 < \rho_2 < \rho_1 < \psi$

$$\varepsilon'^2 = 4\gamma\vartheta'$$
$$\varepsilon^2 - 4\gamma\vartheta > 0$$
$$2\gamma\vartheta > \varepsilon'\left(\varepsilon - \frac{\varepsilon'}{2}\right)$$
$$2\gamma < \varepsilon < \varepsilon'$$
$$(\gamma - \varepsilon + \vartheta) > 0$$

f1] $0<\rho_2<\psi<\rho_1<1,$

$$\varepsilon'^2=4\gamma\vartheta'$$
$$2\gamma\vartheta<\varepsilon'\left(\varepsilon-\frac{\varepsilon'}{2}\right)$$
$$\gamma>\sup\left\{\frac{\varepsilon}{2},\ (\varepsilon-\vartheta)\right\}$$

f2] $0<\rho_2<\psi<1<\rho_1$

$$\varepsilon'^2=4\gamma\vartheta'$$
$$2\gamma\vartheta<\varepsilon'\left(\varepsilon-\frac{\varepsilon'}{2}\right)$$
$$\frac{\varepsilon'}{2}<\gamma<(\varepsilon-\vartheta)$$

f3] $0<\rho_2<1<\psi<\rho_1,$

$$\varepsilon'^2=4\gamma\vartheta'$$
$$2\gamma\vartheta<\varepsilon'\left(\varepsilon-\frac{\varepsilon'}{2}\right)$$
$$\gamma<\inf\left\{\frac{\varepsilon'}{2},(\varepsilon-\vartheta)\right\}$$

f4] $1<\rho_2<\psi<\rho_1,$

$$\varepsilon'^2=4\gamma\vartheta'$$
$$2\gamma\vartheta<\varepsilon'\left(\varepsilon-\frac{\varepsilon'}{2}\right)$$
$$(\varepsilon-\vartheta)<\gamma<\frac{\varepsilon}{2}$$

g1] $0<\rho<\psi<1$

$$\varepsilon^2=4\gamma\vartheta,$$
$$\varepsilon'^2=4\gamma\vartheta'$$
$$\varepsilon<\varepsilon'<2\gamma$$

g2] $0<\rho<1<\psi$

$$\varepsilon^2=4\gamma\vartheta,$$
$$\varepsilon'^2=4\gamma\vartheta'$$
$$\varepsilon<2\gamma<\varepsilon'$$

g3] $1<\rho<\psi$

$$\varepsilon^2=4\gamma\vartheta,$$
$$\varepsilon'^2=4\gamma\vartheta'$$
$$2\gamma<\varepsilon<\varepsilon'$$

h1] $0<\psi<\rho<1$

$$\varepsilon^2=4\gamma\vartheta$$
$$\varepsilon'^2=4\gamma\vartheta'$$
$$\varepsilon'<\varepsilon<2\gamma$$

h2] $0<\psi<1<\rho$

$$\varepsilon^2=4\gamma\vartheta$$
$$\varepsilon'^2=4\gamma\vartheta'$$
$$\varepsilon'<2\gamma<\varepsilon$$

h3] $1<\psi<\rho$

$$\varepsilon^2=4\gamma\vartheta$$
$$\varepsilon'^2=4\gamma\vartheta'$$
$$2\gamma<\varepsilon'<\varepsilon$$

i1] $0<\rho=\psi<1$

$$\varepsilon^2=4\gamma\vartheta$$
$$\varepsilon'^2=4\gamma\vartheta'$$
$$\varepsilon=\varepsilon'<2\gamma$$

i2] $1<\rho=\psi$

$$\varepsilon^2=4\gamma\vartheta$$
$$\varepsilon'^2=4\gamma\vartheta'$$
$$\varepsilon=\varepsilon'>2\gamma$$

CASE C

a1] ρ_1, ρ_2 are complex and $0 < \Psi_2 < \Psi_1 < 1$

$\varepsilon^2 < 4\gamma\vartheta$,
$\varepsilon'^2 > 4\gamma\vartheta'$
$\gamma > \sup\{\frac{\varepsilon'}{2}, (\varepsilon'-\vartheta')\}$

a2] ρ_1, ρ_2 are complex and $0 < \Psi_2 < 1 < \Psi_1$

$\varepsilon^2 < 4\gamma\vartheta$
$(\gamma-\varepsilon'+\vartheta') < 0$

a3] ρ_1, ρ_2 are complex and $1 < \Psi_2 < \Psi_1$

$\varepsilon^2 < 4\gamma\vartheta$
$\varepsilon'^2 > 4\gamma\vartheta'$
$(\varepsilon'-\vartheta') < \gamma < \frac{\varepsilon'}{2}$

b1] ρ_1, ρ_2 are complex and $0 < \Psi < 1$

$\varepsilon^2 < 4\gamma\vartheta$,
$\varepsilon'^2 = 4\gamma\vartheta'$
$\varepsilon' < 2\gamma$

b2] ρ_1, ρ_2 are complex and $1 < \Psi$

$\varepsilon^2 < 4\gamma\vartheta$
$\varepsilon'^2 = 4\gamma\vartheta'$
$\varepsilon' > 2\gamma$

c1] Ψ_1, Ψ_2 are complex and $0 < \rho_2 < \rho_1 < 1$

$\varepsilon'^2 < 4\gamma\vartheta'$
$\varepsilon^2 > 4\gamma\vartheta$
$\gamma > \sup\{\frac{\varepsilon}{2}, (\varepsilon-\vartheta)\}$

c2] Ψ_1, Ψ_2 are complex and $0 < \rho_2 < 1 < \rho_1$

$\varepsilon'^2 < 4\gamma\vartheta'$
$(\gamma-\varepsilon+\vartheta) < 0$

c3] ψ_1, ψ_2 are complex and $1 < \rho_2 < \rho_1$.

$$\varepsilon'^2 < 4\gamma\vartheta'$$
$$\varepsilon^2 > 4\gamma\vartheta$$
$$(\varepsilon-\vartheta) < \gamma < \frac{\varepsilon}{2}$$

d1] ψ_1, ψ_2 are complex and $0 < \rho < 1$

$$\varepsilon'^2 < 4\gamma\vartheta'$$
$$\varepsilon^2 = 4\gamma\vartheta$$
$$\varepsilon < 2\gamma$$

d2] ψ_1, ψ_2 are complex and $1 < \rho$

$$\varepsilon'^2 < 4\gamma\vartheta'$$
$$\varepsilon^2 = 4\gamma\vartheta$$
$$\varepsilon > 2\gamma$$

e] ψ_1 , ψ_2 and ρ_1, ρ_2 are complex.

$$\varepsilon^2 < 4\gamma\vartheta$$
$$\varepsilon'^2 < 4\gamma\vartheta'$$

CHAPTER V

Here we classify the critical points of the linearized system (27) for the special case $k_1[A] = k_2[B]$, for all possible arrangements of the root positions of the polynomials $\Phi(y_s)$ and $G(y_s)$, by using theorem 3.1.

Va] Introduction

According to theorem 3.1, we need to know the sign of $\det\underline{A}$ and $\mathrm{tr}\underline{A}$ in order to classify the critical points of the linearized system (27). For the special case $k_1[A] = k_2[B]$, we were able to derive the polynomials $\Phi(y_s)$ and $G(y_s)$ which have the same sign as $\det\underline{A}$ and $\mathrm{tr}\underline{A}$, respectively. Now, the sign of $\Phi(y_s)$ and $G(y_s)$ depends on the position of $y_s \in (0,1)$ with respect to ρ_1, ρ_2, Ψ_1, Ψ_2, as well as on the nature of these roots. In the previous chapter, we distinguished cases (A)-(C) according to the nature of the roots ρ_1, ρ_2, Ψ_1, Ψ_2; for these cases we obtained a large number of possible arrangements of the root positions, and derived the necessary and sufficient conditions for each arrangement.

Next, we show that for each possible arrangement of the root positions a number of subcases can be distinguished depending on the magnitude of $y_s \in (0,1)$, and that in each subcase the sign of $\Phi(y_s)$ and $G(y_s)$ can be determined and the critical points classified. Recall that $\Phi(y_s)$ and $G(y_s)$ are given by

$$\Phi(y_s) = \gamma y_s^2 - \varepsilon y_s + \vartheta \tag{40}$$

$$G(y_s) = -\gamma y_s^2 + \varepsilon' y_s - \vartheta' \tag{41}$$

where $\gamma > 0$. For the special case $k_1[A] = k_2[B]$, the critical points are roots of the equation

$$K_3^\circ y_s^2 e^{-\mu y_s} + \left\{K_{-1} + K_1[A]\left(1 + \frac{K_{-1}}{K_{-2}}\right)\right\} y_s - K_1[A]\left(\frac{K_{-1}}{K_{-2}}\right) = 0 \tag{47}$$

where $y_s \in (0,1)$.

Vb] Classification of the critical points for the special case $k_1[A] = k_2[B]$.

For cases (A)-(C), we classify all possible arrangements for the root positions, taking into account the magnitude of $y_s \in (0,1)$. This allows us to determine the sign of $\Phi(y_s)$ and $G(y_s)$, so that we can classify the critical points by using theorem 3.1. The results of this classification are presented in tabular form for each group listed; for the "type of steady state" we use the notation:

1: Stable focus (or stable node).

2: Unstable focus (or unstable node).

3: Saddle point.

CASE A

Table 5.1

	Arrangement	Sign of $\Phi(y_s)$	Sign of $G(y_s)$	Type of Steady State
a11	$0<\rho_2<\Psi_2<\rho_1<\Psi_1<y_s<1$	+	-	1
a12	$0<\rho_2<\Psi_2<\rho_1<y_s<\Psi_1<1$	+	+	2
a13	$0<\rho_2<\Psi_2<y_s<\rho_1<\Psi_1<1$	-	+	3
a14	$0<\rho_2<y_s<\Psi_2<\rho_1<\Psi_1<1$	-	-	3
a15	$0<y_s<\rho_2<\Psi_2<\rho_1<\Psi_1<1$	+	-	1
a21	$0<\rho_2<\Psi_2<\rho_1<y_s<1<\Psi_1$	+	+	2
a22	$0<\rho_2<\Psi_2<y_s<\rho_1<1<\Psi_1$	-	+	3
a23	$0<\rho_2<y_s<\Psi_2<\rho_1<1<\Psi_1$	-	-	3
a24	$0<y_s<\rho_2<\Psi_2<\rho_1<1<\Psi_1$	+	-	1
a31	$0<\rho_2<\Psi_2<y_s<1<\rho_1<\Psi_1$	-	+	3
a32	$0<\rho_2<y_s<\Psi_2<1<\rho_1<\Psi_1$	-	-	3
a33	$0<y_s<\rho_2<\Psi_2<1<\rho_1<\Psi_1$	+	-	1
a41	$0<\rho_2<y_s<1<\Psi_2<\rho_1<\Psi_1$	-	-	3
a42	$0<y_s<\rho_2<1<\Psi_2<\rho_1<\Psi_1$	+	-	1
a5	$0<y_s<1<\rho_2<\Psi_2<\rho_1<\Psi_1$	+	-	1

Table 5.2

	Arrangement	Sign of $\Phi(y_s)$	Sign of $G(y_s)$	Type of Steady State
b11	$0<\Psi_2<\rho_2<\Psi_1<\rho_1<y_s<1$	+	-	1
b12	$0<\Psi_2<\rho_2<\Psi_1<y_s<\rho_1<1$	-	-	3
b13	$0<\Psi_2<\rho_2<y_s<\Psi_1<\rho_1<1$	-	+	3
b14	$0<\Psi_2<y_s<\rho_2<\Psi_1<\rho_1<1$	+	+	2
b15	$0<y_s<\Psi_2<\rho_2<\Psi_1<\rho_1<1$	+	-	1
b21	$0<\Psi_2<\rho_2<\Psi_1<y_s<1<\rho_1$	-	-	3
b22	$0<\Psi_2<\rho_2<y_s<\Psi_1<1<\rho_1$	-	+	3
b23	$0<\Psi_2<y_s<\rho_2<\Psi_1<1<\rho_1$	+	+	2
b24	$0<y_s<\Psi_2<\rho_2<\Psi_1<1<\rho_1$	+	-	1
b31	$0<\Psi_2<\rho_2<y_s<1<\Psi_1<\rho_1$	-	+	3
b32	$0<\Psi_2<y_s<\rho_2<1<\Psi_1<\rho_1$	+	+	2
b33	$0<y_s<\Psi_2<\rho_2<1<\Psi_1<\rho_1$	+	-	1
b41	$0<\Psi_2<y_s<1<\rho_2<\Psi_1<\rho_1$	+	+	2
b42	$0<y_s<\Psi_2<1<\rho_2<\Psi_1<\rho_1$	+	-	1
b5	$0<y_s<1<\Psi_2<\rho_2<\Psi_1<\rho_1$	+	-	1

Table 5.3

	Arrangement	Sign of $\Phi(y_s)$	Sign of $G(y_s)$	Type of Steady State
c11	$0<\rho_2<\Psi_2<\Psi_1<\rho_1<y_s<1$	+	-	1
c12	$0<\rho_2<\Psi_2<\Psi_1<y_s<\rho_1<1$	-	-	3
c13	$0<\rho_2<\Psi_2<y_s<\Psi_1<\rho_1<1$	-	+	3
c14	$0<\rho_2<y_s<\Psi_2<\Psi_1<\rho_1<1$	-	-	3
c15	$0<y_s<\rho_2<\Psi_2<\Psi_1<\rho_1<1$	+	-	1
c21	$0<\rho_2<\Psi_2<\Psi_1<y_s<1<\rho_1$	-	-	3
c22	$0<\rho_2<\Psi_2<y_s<\Psi_1<1<\rho_1$	-	+	3
c23	$0<\rho_2<y_s<\Psi_2<\Psi_1<1<\rho_1$	-	-	3
c24	$0<y_s<\rho_2<\Psi_2<\Psi_1<1<\rho_1$	+	-	1
c31	$0<\rho_2<\Psi_2<y_s<1<\Psi_1<\rho_1$	-	+	3
c32	$0<\rho_2<y_s<\Psi_2<1<\Psi_1<\rho_1$	-	-	3
c33	$0<y_s<\rho_2<\Psi_2<1<\Psi_1<\rho_1$	+	-	1
c41	$0<\rho_2<y_s<1<\Psi_2<\Psi_1<\rho_1$	-	-	3
c42	$0<y_s<\rho_2<1<\Psi_2<\Psi_1<\rho_1$	+	-	1
c5	$0<y_s<1<\rho_2<\Psi_2<\Psi_1<\rho_1$	+	-	1

Table 5.4

	Arrangement	Sign of $\Phi(y_s)$	Sign of $G(y_s)$	Type of Steady State
d11	$0<\Psi_2<\rho_2<\rho_1<\Psi_1<y_s<1$	+	-	1
d12	$0<\Psi_2<\rho_2<\rho_1<y_s<\Psi_1<1$	+	+	2
d13	$0<\Psi_2<\rho_2<y_s<\rho_1<\Psi_1<1$	-	+	3
d14	$0<\Psi_2<y_s<\rho_2<\rho_1<\Psi_1<1$	+	+	2
d15	$0<y_s<\Psi_2<\rho_2<\rho_1<\Psi_1<1$	+	-	1
d21	$0<\Psi_2<\rho_2<\rho_1<y_s<1<\Psi_1$	+	+	2
d22	$0<\Psi_2<\rho_2<y_s<\rho_1<1<\Psi_1$	-	+	3
d23	$0<\Psi_2<y_s<\rho_2<\rho_1<1<\Psi_1$	+	+	2
d24	$0<y_s<\Psi_2<\rho_2<\rho_1<1<\Psi_1$	+	-	1
d31	$0<\Psi_2<\rho_2<y_s<1<\rho_1<\Psi_1$	-	+	3
d32	$0<\Psi_2<y_s<\rho_2<1<\rho_1<\Psi_1$	+	+	2
d33	$0<y_s<\Psi_2<\rho_2<1<\rho_1<\Psi_1$	+	-	1
d41	$0<\Psi_2<y_s<1<\rho_2<\rho_1<\Psi_1$	+	+	2
d42	$0<y_s<\Psi_2<1<\rho_2<\rho_1<\Psi_1$	+	-	1
d5	$0<y_s<1<\Psi_2<\rho_2<\rho_1<\Psi_1$	+	-	1

Table 5.5

	Arrangement	Sign of $\Phi(y_s)$	Sign of $G(y_s)$	Type of Steady State
e11	$0<\rho_2<\rho_1<\Psi_2<\Psi_1<y_s<1$	+	-	1
e12	$0<\rho_2<\rho_1<\Psi_2<y_s<\Psi_1<1$	+	+	2
e13	$0<\rho_2<\rho_1<y_s<\Psi_2<\Psi_1<1$	+	-	1
e14	$0<\rho_2<y_s<\rho_1<\Psi_2<\Psi_1<1$	-	-	3
e15	$0<y_s<\rho_2<\rho_1<\Psi_2<\Psi_1<1$	+	-	1
e21	$0<\rho_2<\rho_1<\Psi_2<y_s<1<\Psi_1$	+	+	2
e22	$0<\rho_2<\rho_1<y_s<\Psi_2<1<\Psi_1$	+	-	1
e23	$0<\rho_2<y_s<\rho_1<\Psi_2<1<\Psi_1$	-	-	3
e24	$0<y_s<\rho_2<\rho_1<\Psi_2<1<\Psi_1$	+	-	1
e31	$0<\rho_2<\rho_1<y_s<1<\Psi_2<\Psi_1$	+	-	1
e32	$0<\rho_2<y_s<\rho_1<1<\Psi_2<\Psi_1$	-	-	3
e33	$0<y_s<\rho_2<\rho_1<1<\Psi_2<\Psi_1$	+	-	1
e41	$0<\rho_2<y_s<1<\rho_1<\Psi_2<\Psi_1$	-	-	3
e42	$0<y_s<\rho_2<1<\rho_1<\Psi_2<\Psi_1$	+	-	1
e5	$0<y_s<1<\rho_2<\rho_1<\Psi_2<\Psi_1$	+	-	1

Table 5.6

	Arrangement	Sign of $\Phi(y_s)$	Sign of $G(y_s)$	Type of Steady State
f11	$0<\Psi_2<\Psi_1<\rho_2<\rho_1<y_s<1$	+	-	1
f12	$0<\Psi_2<\Psi_1<\rho_2<y_s<\rho_1<1$	-	-	3
f13	$0<\Psi_2<\Psi_1<y_s<\rho_2<\rho_1<1$	+	-	1
f14	$0<\Psi_2<y_s<\Psi_1<\rho_2<\rho_1<1$	+	+	2
f15	$0<y_s<\Psi_2<\Psi_1<\rho_2<\rho_1<1$	+	-	1
f21	$0<\Psi_2<\Psi_1<\rho_2<y_s<1<\rho_1$	-	-	3
f22	$0<\Psi_2<\Psi_1<y_s<\rho_2<1<\rho_1$	+	-	1
f23	$0<\Psi_2<y_s<\Psi_1<\rho_2<1<\rho_1$	+	+	2
f24	$0<y_s<\Psi_2<\Psi_1<\rho_2<1<\rho_1$	+	-	1
f31	$0<\Psi_2<\Psi_1<y_s<1<\rho_2<\rho_1$	+	-	1
f32	$0<\Psi_2<y_s<\Psi_1<1<\rho_2<\rho_1$	+	+	2
f33	$0<y_s<\Psi_2<\Psi_1<1<\rho_2<\rho_1$	+	-	1
f41	$0<\Psi_2<y_s<1<\Psi_1<\rho_2<\rho_1$	+	+	2
f42	$0<y_s<\Psi_2<1<\Psi_1<\rho_2<\rho_1$	+	-	1
f5	$0<y_s<1<\Psi_2<\Psi_1<\rho_2<\rho_1$	+	-	1

CASE B

Table 5.7

	Arrangement	Sign of $\Phi(y_s)$	Sign of $G(y_s)$	Type of Steady State
a11	$0<\rho<\Psi_2<\Psi_1<y_s<1$	+	-	1
a12	$0<\rho<\Psi_2<y_s<\Psi_1<1$	+	+	2
a13	$0<\rho<y_s<\Psi_2<\Psi_1<1$	+	-	1
a14	$0<y_s<\rho<\Psi_2<\Psi_1<1$	+	-	1
a21	$0<\rho<\Psi_2<y_s<1<\Psi_1$	+	+	2
a22	$0<\rho<y_s<\Psi_2<1<\Psi_1$	+	-	1
a23	$0<y_s<\rho<\Psi_2<1<\Psi_1$	+	-	1
a31	$0<\rho<y_s<1<\Psi_2<\Psi_1$	+	-	1
a32	$0<y_s<\rho<1<\Psi_2<\Psi_1$	+	-	1
a4	$0<y_s<1<\rho<\Psi_2<\Psi_1$	+	-	1
b11	$0<\Psi_2<\Psi_1<\rho<y_s<1$	+	-	1
b12	$0<\Psi_2<\Psi_1<y_s<\rho<1$	+	-	1
b13	$0<\Psi_2<y_s<\Psi_1<\rho<1$	+	+	2
b14	$0<y_s<\Psi_2<\Psi_1<\rho<1$	+	-	1
b21	$0<\Psi_2<\Psi_1<y_s<1<\rho$	+	-	1
b22	$0<\Psi_2<y_s<\Psi_1<1<\rho$	+	+	2
b23	$0<y_s<\Psi_2<\Psi_1<1<\rho$	+	-	1
b31	$0<\Psi_2<y_s<1<\Psi_1<\rho$	+	+	2
b32	$0<y_s<\Psi_2<1<\Psi_1<\rho$	+	-	1
b4	$0<y_s<1<\Psi_2<\Psi_1<\rho$	+	-	1

Table 5.8

	Arrangement	Sign of $\Phi(y_s)$	Sign of $G(y_s)$	Type of Steady State
c11	$0<\Psi_2<\rho<\Psi_1<y_s<1$	+	-	1
c12	$0<\Psi_2<\rho<y_s<\Psi_1<1$	+	+	2
c13	$0<\Psi_2<y_s<\rho<\Psi_1<1$	+	+	2
c14	$0<y_s<\Psi_2<\rho<\Psi_1<1$	+	-	1
c21	$0<\Psi_2<\rho<y_s<1<\Psi_1$	+	+	2
c22	$0<\Psi_2<y_s<\rho<1<\Psi_1$	+	+	2
c23	$0<y_s<\Psi_2<\rho<1<\Psi_1$	+	-	1
c31	$0<\Psi_2<y_s<1<\rho<\Psi_1$	+	+	2
c32	$0<y_s<\Psi_2<1<\rho<\Psi_1$	+	-	1
c4	$0<y_s<1<\Psi_2<\rho<\Psi_1$	+	-	1
d11	$0<\Psi<\rho_2<\rho_1<y_s<1$	+	-	1
d12	$0<\Psi<\rho_2<y_s<\rho_1<1$	-	-	3
d13	$0<\Psi<y_s<\rho_2<\rho_1<1$	+	-	1
d14	$0<y_s<\Psi<\rho_2<\rho_1<1$	+	-	1
d21	$0<\Psi<\rho_2<y_s<1<\rho_1$	-	-	3
d22	$0<\Psi<y_s<\rho_2<1<\rho_1$	+	-	1
d23	$0<y_s<\Psi<\rho_2<1<\rho_1$	+	-	1
d31	$0<\Psi<y_s<1<\rho_2<\rho_1$	+	-	1
d32	$0<y_s<\Psi<1<\rho_2<\rho_1$	+	-	1
d4	$0<y_s<1<\Psi<\rho_2<\rho_1$	+	-	1

Table 5.9

	Arrangement	Sign of $\Phi(y_s)$	Sign of $G(y_s)$	Type of Steady State
e11	$0<\rho_2<\rho_1<\Psi<y_s<1$	+	-	1
e12	$0<\rho_2<\rho_1<y_s<\Psi<1$	+	-	1
e13	$0<\rho_2<y_s<\rho_1<\Psi<1$	-	-	3
e14	$0<y_s<\rho_2<\rho_1<\Psi<1$	+	-	1
e21	$0<\rho_2<\rho_1<y_s<1<\Psi$	+	-	1
e22	$0<\rho_2<y_s<\rho_1<1<\Psi$	-	-	3
e23	$0<y_s<\rho_2<\rho_1<1<\Psi$	+	-	1
e31	$0<\rho_2<y_s<1<\rho_1<\Psi$	-	-	3
e32	$0<y_s<\rho_2<1<\rho_1<\Psi$	+	-	1
e4	$0<y_s<1<\rho_2<\rho_1<\Psi$	+	-	1
f11	$0<\rho_2<\Psi<\rho_1<y_s<1$	+	-	1
f12	$0<\rho_2<\Psi<y_s<\rho_1<1$	-	-	3
f13	$0<\rho_2<y_s<\Psi<\rho_1<1$	-	-	3
f14	$0<y_s<\rho_2<\Psi<\rho_1<1$	+	-	1
f21	$0<\rho_2<\Psi<y_s<1<\rho_1$	-	-	3
f22	$0<\rho_2<y_s<\Psi<1<\rho_1$	-	-	3
f23	$0<y_s<\rho_2<\Psi<1<\rho_1$	+	-	1
f31	$0<\rho_2<y_s<1<\Psi<\rho_1$	-	-	3
f32	$0<y_s<\rho_2<1<\Psi<\rho_1$	+	-	1
f4	$0<y_s<1<\rho_2<\Psi<\rho_1$	+	-	1

Table 5.10

	Arrangement	Sign of $\Phi(y_s)$	Sign of $G(y_s)$	Type of Steady State
g1	$0<\rho<\Psi<1$	+	-	1
g2	$0<\rho<1<\Psi$	+	-	1
g3	$1<\rho<\Psi$	+	-	1
h1	$0<\Psi<\rho<1$	+	-	1
h2	$0<\Psi<1<\rho$	+	-	1
h3	$1<\Psi<\rho$	+	-	1
i1	$0<\rho=\Psi<1$	+	-	1
i2	$1<\rho=\Psi$	+	-	1

CASE C

Table 5.11

	Arrangement	Sign of $\Phi(y_s)$	Sign of $G(y_s)$	Type of Steady State
a11	ρ_1,ρ_2 are complex and $0<\Psi_2<\Psi_1<y_s<1$	+	-	1
a12	ρ_1,ρ_2 are complex and $0<\Psi_2<y_s<\Psi_1<1$	+	+	2
a13	ρ_1,ρ_2 are complex and $0<y_s<\Psi_2<\Psi_1<1$	+	-	1
a21	ρ_1,ρ_2 are complex and $0<\Psi_2<y_s<1<\Psi_1$	+	+	2
a22	ρ_1,ρ_2 are complex and $0<y_s<\Psi_2<1<\Psi_1$	+	-	1
a3	ρ_1,ρ_2 are complex and $0<y_s<1<\Psi_2<\Psi_1$	+	-	1
b1	ρ_1,ρ_2 are complex and $0<\Psi<1$	+	-	1
b2	ρ_1,ρ_2 are complex and $1<\Psi$	+	-	1
c11	Ψ_1,Ψ_2 are complex and $0<\rho_2<\rho_1<y_s<1$	+	-	1
c12	Ψ_1,Ψ_2 are complex and $0<\rho_2<y_s<\rho_1<1$	-	-	3
c13	Ψ_1,Ψ_2 are complex and $0<y_s<\rho_2<\rho_1<1$	+	-	1
c21	Ψ_1,Ψ_2 are complex and $0<\rho_2<y_s<1<\rho_1$	-	-	3
c22	Ψ_1,Ψ_2 are complex and $0<y_s<\rho_2<1<\rho_1$	+	-	1
c3	Ψ_1,Ψ_2 are complex and $0<y_s<1<\rho_2<\rho_1$	+	-	1
d1	Ψ_1,Ψ_2 are complex and $0<\rho<1$	+	-	1
d2	Ψ_1,Ψ_2 are complex and $1<\rho$	+	-	1
e	Ψ_1,Ψ_2 and ρ_1,ρ_2 are complex	+	-	1

From these tables we see that the steady state will be an unstable focus (or an unstable node) only in the following cases:

TABLE	CASE	ARRANGEMENT
5.1	A	a12, a21
5.2	A	b14, b23, b32, b41
5.4	A	d12, d14, d21, d23, d32, d41
5.5	A	e12, e21
5.6	A	f14, f23, f32, f41
5.7	B	a12, a21, b13, b22, b31
5.8	B	c12, c13, c21, c22, c31
5.11	C	a12, a21

If the steady state is unique, then sustained oscillations will be observed for each of the above arrangements. Necessary and sufficient conditions for uniqueness can be derived.

In the case of multiple steady states, the fact that a critical point is an unstable focus (or an unstable node) does not necessarily mean that limit cycles exist. The only way to investigate this problem is by integrating numerically the dynamic equations.

CHAPTER VI

Uniqueness Criteria

Here, we derive the conditions under which a unique steady state solution exists for a lumped system described by the nonlinear algebraic equation

$$y_s(y_s-\beta_2)e^{-\mu y_s} = \frac{\beta_1 K_1[A](1-\beta_2)+\beta_2[K_{-1}+K_1[A](1+\beta_1)]}{K_3^o} - \frac{[K_{-1}+K_1[A](1+\beta_1)]y_s}{K_3^o} \qquad (14)$$

Multiplication of both sides of the above equation by

$$K_3^o/[K_{-1}+K_1[A](1+\beta_1)]$$

yields,

$$\frac{K_3^o y_s(y_s-\beta_2)e^{-\mu y_s}}{[K_{-1}+K_1[A](1+\beta_1)]} = \left\{\beta_2+\frac{\beta_1 K_1[A](1-\beta_2)}{[K_{-1}+K_1[A](1+\beta_1)]}\right\}-y_s \qquad (56)$$

Let

$$\delta \equiv \left\{\beta_2+\frac{\beta_1 K_1[A](1-\beta_2)}{[K_{-1}+K_1[A](1+\beta_1)]}\right\} \qquad (57)$$

But according to (12a),

$$\beta_1 = \frac{\{K_{-1}+K_1[A]-K_2[B]\}}{\{K_{-2}-K_1[A]+K_2[B]\}}, \quad \beta_2 = \left\{\frac{K_2[B]-K_1[A]}{K_{-2}-K_1[A]+K_2[B]}\right\}$$

Substituting in (57), it yields

$$\delta \equiv \frac{K_{-1}K_2[B]}{K_{-1}K_2[B]+K_{-1}K_{-2}+K_{-2}K_1[A]} \qquad (58)$$

where $0 < \delta < 1$.

Using (57), we can write (56) as

$$\frac{K_3^0 y_s(y_s-\beta_2)\, e^{-\mu y_s}}{[K_{-1}+K_1[A](1+\beta_1)]} = (\delta - y_s) \tag{59}$$

or

$$\frac{\{y_s(y_s-\beta_2)e^{-\mu y_s}/[K_{-1}+K_1[A](1+\beta_1)]\}}{(\delta-y_s)} = \frac{1}{K_3^0} \tag{60}$$

Let

$$f(y_s) \equiv \frac{y_s(y_s-\beta_2)\, e^{-\mu y_s}}{[K_{-1}+K_1[A](1+\beta_1)]} \tag{61}$$

and

$$\tau \equiv k_3^0 \tag{62}$$

Then, we can write (60) as

$$F(y_s) = \frac{f(y_s)}{(\delta-y_s)} = \frac{1}{\tau} \tag{63}$$

From (63) we have that

$$(\delta-y_s) = \tau\, f(y_s) \tag{64}$$

where $0 < y_s \neq \delta < 1$.

At this point, we would like to examine the sign of $f(y_s)$ which is defined by (61). We have the following possibilities:

CASE I

Suppose that

$$K_2[B] - K_1[A] > 0$$

Then,

$$\{K_{-2} - K_1[A] + K_2[B]\} > 0$$

Using (12a), we have

$$\left[K_{-1} + K_1[A](1+\beta_1)\right] \equiv \frac{K_{-1}\left(K_{-2}+K_2[B]\right)+K_{-2}K_1[A]}{\left\{K_{-2}-K_1[A]+K_2[B]\right\}} > 0$$

and

$$0 < \beta_2 < 1$$

where

$$\beta_2 = \left\{K_2[B]-K_1[A]\right\} / \left\{K_{-2}-K_1[A]+K_2[B]\right\}$$

Since $0 < y_s < 1$, we cannot draw in this case any conclusions about the sign of ($y_s - \beta_2$). By looking at equ.(60), however, we see that since the right-hand side of this equation is positive, we must have either that

(i) $\beta_2 < y_s < \delta$

or

(ii) $\delta < y_s < \beta_2$

When $\beta_2 < y_s < \delta$, we have that $f(y_s) > 0$.
When $\delta < y_s < \beta_2$, we have that $f(y_s) < 0$.

CASE II

Suppose that

$$K_2[B]-K_1[A] < 0 \qquad (65)$$

Then either $K_{-2}+K_2[B]-K_1[A] < 0$, or we have that

$K_{-2}+K_2[B]-K_1[A] > 0$.

(i) If in addition to (65) we have that $K_{-2}+K_2[B]-K_1[A] < 0$

then

$$[K_{-1}+K_1[A](1+\beta_1)] < 0$$

and

$$\beta_2 > 1$$

As result, $(y_s-\beta_2) < 0$, and, consequently, $f(y_s) > 0$.

(ii) If in addition to (65) we have that

$$K_{-2}+K_2[B]-K_1[A] > 0$$

then

$$[K_{-1}+K_1[A](1+\beta_1)] > 0$$

and

$$\beta_2 < 0$$

As result, $(y_s-\beta_2) > 0$, and, consequently, $f(y_s) > 0$.

CASE III

Suppose that

$$K_2[B]-K_1[A] = 0$$

then

$$[K_{-1}+K_1[A](1+\beta_1)] > 0$$

and

$$\beta_2 = 0$$

As result, $(y_s-\beta_2) > 0$, and, consequently, $f(y_s) > 0$.

Conclusion: $f(y_s) > 0$ for $0 < y_s \neq \delta < 1$, except in case I(ii).

Since $F(y_s) \rightarrow \infty$ as $y_s \rightarrow \delta$, we can distinguish the following possibilities in connection with cases II and III only:

1) $y_s \in (0, \delta)$

2) $y_s \in (\delta, 1)$

In case (1), $(\delta - y_s) > 0$, and the lumped system is described by equ.(64):

$$(\delta - y_s) = \tau f(y_s)$$

In case (2), $(\delta - y_s) < 0$, and the lumped system is described by

$$(y_s - \delta) = -\tau f(y_s)$$

This equation, however, cannot be satisfied, because the left-hand side is positive, while the right-hand side is negative. As result, there are no steady state solutions for $y_s \in (\delta, 1)$ in cases II and III.

Now, we will develop uniqueness criteria for cases I-III.

CASE I

(i) Here we have that $\beta_2 < y_s < \delta$. If the function

$$F(y_s) = f(y_s)/(\delta - y_s)$$

is monotonic, a unique solution exists. Hence, a necessary and sufficient condition for uniqueness for all τ is that

$$\frac{d}{dy_s}\left(\frac{f(y_s)}{\delta - y_s}\right) > 0$$

Differentiating and multiplying by $(\delta - y_s)^2$, we have

$$(\delta - y_s) f'(y_s) + f(y_s) > 0$$

and $$(\delta - y_s) f'(y_s) > -f(y_s)$$

dividing both sides by $f(y_s) > 0$, it yields

$$\frac{(\delta - y_s) f'(y_s)}{f(y_s)} > -1$$

and since

$$\frac{d \ln f(y_s)}{d y_s} = \frac{1}{f(y_s)} \frac{d f(y_s)}{d y_s} = \frac{f'(y_s)}{f(y_s)}$$

we can rewrite it as

$$(\delta - y_s) \frac{d \ln f(y_s)}{d y_s} > -1$$

Taking the logarithm of both sides of

$$f(y_s) = \frac{y_s (y_s - \beta_2)\, e^{-\mu y_s}}{[K_{-1} + K_1 [A](1+\beta_1)]}$$

we have that

$$\ln f(y_s) = \ln [y_s (y_s - \beta_2)] - \mu y_s - \ln [K_{-1} + K_1 [A](1+\beta_1)]$$

and differentiating,

$$\frac{d \ln [f(y_s)]}{d y_s} = \frac{(2 y_s - \beta_2)}{y_s (y_s - \beta_2)} - \mu$$

Thus, the necessary and sufficient condition for all τ is

$$(\delta - y_s) \left[\frac{(2 y_s - \beta_2)}{y_s (y_s - \beta_2)} - \mu \right] > -1$$

or

$$\frac{(\delta - y_s)(2 y_s - \beta_2)}{y_s (y_s - \beta_2)} > -1 + \mu (\delta - y_s)$$

Multiplying both sides of this inequality by y_s, it yields

$$\frac{(\delta-y_s)(2y_s-\beta_2)}{(y_s-\beta_2)} > -y_s + \mu y_s(\delta-y_s)$$

Consequently,

$$-2y_s + (2\delta-\beta_2) + \frac{\beta_2(\delta-\beta_2)}{(y_s-\beta_2)} > -y_s + \mu y_s(\delta-y_s)$$

or

$$\mu y_s^2 - (1+\mu\delta)y_s + 2\delta > \frac{\beta_2(y_s-\delta)}{(y_s-\beta_2)} \qquad (78)$$

Since $(y_s-\beta_2)>0$, we can multiply both sides of (78) by this term to get

$$-\beta_2\delta + \delta(2+\mu\beta_2)y_s - [1+\mu(\beta_2+\delta)]y_s^2 + \mu y_s^3 > 0$$

Now, making the substitution

$$0 < \sigma \equiv \frac{(y_s-\beta_2)}{(\delta-\beta_2)} < 1$$

we can rewrite the above inequality as

$$A(\sigma) \equiv b_0 + b_1\sigma + b_2\sigma^2 + b_3\sigma^3 > 0$$

where

$$b_0 \equiv \beta_2$$

$$b_1 \equiv (\delta-\beta_2)(2-\mu\beta_2)$$

$$b_2 \equiv (\delta-\beta_2)[\mu(2\beta_2-\delta)-1]$$

$$b_3 \equiv \mu(\delta-\beta_2)^2$$

Sufficient conditions for $A(\sigma)>0$, whenever $0<\sigma<1$, are according to [17]

$$b_0 \equiv \beta_2 > 0$$
$$b_1 + 3b_0 > 0$$
$$b_1 + b_2 > 0$$
$$b_2 + 3b_3 > 0$$

Substituting, we have that the sufficient conditions for uniqueness for all τ are in this case:

$$\frac{1}{(2\delta - \beta_2)} < \mu < \frac{1}{(\delta - \beta_2)}$$

(ii) Here we have that $\delta < y_s < \beta_2$, and $f(y_s) < 0$.
Again, if the function

$$F(y_s) = f(y_s) / (\delta - y_s)$$

is monotonic, a unique solution exists. Hence, a necessary and sufficient condition for uniqueness for all τ is

$$\frac{d}{dy_s}\left(\frac{f(y_s)}{\delta - y_s}\right) < 0$$

Following the same procedure as in case I(i), we arrive at equ.(78). Multiplying both sides of (78) by $(y_s - \beta_2) < 0$, we get

$$-\beta_2\delta + \delta(2 + \mu\beta_2)y_s - [1 + \mu(\beta_2 + \delta)]y_s^2 + \mu y_s^3 < 0$$

Making the substitution

$$0 < w \equiv \frac{(y_s - \delta)}{(\beta_2 - \delta)} < 1$$

and multiplying both sides by minus one we arrive at

$$B(w) \equiv b_0^* + b_1^* w + b_2^* w^2 + b_3^* w^3 > 0$$

where

$$b_0^* \equiv \delta$$
$$b_1^* \equiv \mu\delta(\beta_2 - \delta) \quad .$$
$$b_2^* \equiv (\beta_2 - \delta)\left[-\mu(2\delta - \beta_2) + 1\right]$$
$$b_3^* \equiv -\mu(\beta_2 - \delta)^2$$

Sufficient conditions for uniqueness for all τ are in this case[17]:

$$0 < \mu < \frac{1}{(2\beta_2 - \delta)}$$

Remark: In case I, it is impossible to have $\beta_2 = \delta$.

CASE II

(i). Here we have that $\beta_2 > 1$, and $(y_s - \beta_2) < 0$. Multiplying both sides of (78) by $-(y_s - \beta_2)$ it yields

$$Z(y_s) \equiv a_0' + a_1' y_s + a_2' y_s^2 + a_3' y_s^3 > 0$$

where $y_s \in (0, \delta)$, and

$$a_0' \equiv \beta_2 \delta$$
$$a_1' \equiv -\delta(2 + \mu\beta_2)$$
$$a_2' \equiv \left[1 + \mu(\beta_2 + \delta)\right]$$
$$a_3' \equiv -\mu$$

The above inequality can be rewritten as

$$Z(\sigma') \equiv a_0^* + a_1^* \sigma' + a_2^* \sigma'^2 + a_3^* \sigma'^3 > 0$$

where

$$0 < \sigma' \equiv \frac{y_s}{\delta} < 1$$

and

$$a_0^* \equiv \beta_2 \delta$$
$$a_1^* \equiv -\delta^2 (2 + \mu \beta_2)$$
$$a_2^* \equiv \delta^2 [1 + \mu(\beta_2 + \delta)]$$
$$a_3^* \equiv -\mu \delta^3$$

Sufficient conditions for $Z(\sigma') > 0$, whenever $\sigma' \in (0,1)$, are according to [17]:

$$a_0^* > 0$$

$$\nu a_\nu^* + (n - \nu + 1) a_{\nu-1}^* > 0 \quad , \quad (\nu = 1, \ldots, n)$$

where n is the degree of $Z(\sigma')$.

The first condition is automatically satisfied, the second condition can be written in its full form as

$$a_1^* + 3a_0^* > 0$$
$$a_1^* + a_2^* > 0$$
$$a_2^* + 3a_3^* > 0$$

Substituting, we can write these conditions as

$$\frac{1}{\delta} < \mu < \left(\frac{3}{\delta} - \frac{2}{\beta_2}\right)$$

$$\mu(2\delta-\beta_2)<1$$

In a better form, we can write that the sufficient conditions for uniqueness for all τ in this case are:

$$\frac{1}{\delta}<\mu<\left(\frac{3}{\delta}-\frac{2}{\beta_2}\right), \quad (2\delta-\beta_2)<\frac{1}{\mu}$$

(ii) Here we have that $\beta_2<0$ and $(y_s-\beta_2)>0$. Multiplying both sides of (78) by $(y_s-\beta_2)$ it yields

$$\Omega(\sigma')\equiv a_0+a_1\sigma'+a_2\sigma'^2+a_3\sigma'^3>0$$

where

$$0<\sigma'\equiv\frac{y_s}{\delta}<1$$

and

$$a_0\equiv-\beta_2\delta$$
$$a_1\equiv\delta^2(2+\mu\beta_2)$$
$$a_2\equiv-\delta^2[1+\mu(\beta_2+\delta)]$$
$$a_3\equiv\mu\delta^3$$

Similarly, we can derive sufficient conditions for uniqueness for all τ [17]:

$$\left(\frac{3}{\delta}-\frac{2}{\beta_2}\right)<\mu<\frac{1}{\delta}$$

$$(2\delta-\beta_2)>\frac{1}{\mu}$$

CASE III

Here we have that $\beta_2 \equiv 0$. Then equ. (78) becomes

$$\mu y_s^2 - (1+\mu\delta) y_s + 2\delta > 0 \tag{108}$$

Recall also that $y_s \in (0,\delta)$.

Let

$$A(y_s) \equiv \mu y_s^2 - (1+\mu\delta) y_s + 2\delta$$

and σ_1, σ_2 be the roots of $A(y_s)=0$.

Then,

$$\sigma_1 = \frac{(1+\mu\delta) - \sqrt{(1-\mu\delta)^2 - 4\mu\delta}}{2\mu}$$

$$\sigma_2 = \frac{(1+\mu\delta) + \sqrt{(1-\mu\delta)^2 - 4\mu\delta}}{2\mu}$$

In connection with the sign of the discriminant

$$\Delta = (1-\mu\delta)^2 - 4\mu\delta$$

we can distinguish the following subcases:

a) $$(1-\mu\delta)^2 < 4\mu\delta \tag{109}$$

Then $A(y_s) > 0$ for any real value of y_s. Thus, the condition $(1-\mu\delta)^2 < 4\mu\delta$ is a sufficient condition for (108) to hold.

b) $(1-\mu\delta)^2 = 4\mu\delta$

Then $\sigma_1 = \sigma_2 = \dfrac{(1+\mu\delta)}{2\mu}$, and $A(y_s) > 0$ if in addition we have that $\mu < \frac{1}{\delta}$.

c) $(1-\mu\delta)^2 > 4\mu\delta$

Then σ_1, σ_2 are real and unequal; in fact, we can prove that they are positive.

Now, we can distinguish the following subcases:

(1) Suppose that $\mu < \frac{1}{\delta}$; then, we have that $A(y_s) > 0$.

(2) Suppose that $\mu > 1/\delta$. Then, $\sigma_1, \sigma_2 \in (0, \delta)$.

CHAPTER VII

Here we present sets of parameter values for which the dynamic equations, when numerically integrated, give rise to limit cycles. These values are such that a unique steady state solution exists for equ.(14), when $k_1[A] = k_2[B]$.

VIIa] Kinetic parameter values

In this study, our purpose is to prove the existence of oscillatory solutions for some values of the kinetic parameters. In other words, we need to find parameter values for which the dynamic equations give rise to limit cycles. For simplicity, we restrict our search by choosing values such that $k_1[A] = k_2[B]$, and for which (109) -the sufficient condition for uniqueness for all τ- is satisfied.

For a unique steady state solution for which $k_1[A] = k_2[B]$, the dynamic equations give rise to limit cycles, if the kinetic parameter values are such that

$$\det \underline{A} > 0$$

$$\mathrm{tr}\,\underline{A} > 0$$

For illustration, we present the following two examples:

EXAMPLE 1

Suppose that

$k_1[A] = k_2[B] = 2.00$

$k_{-1} = 1/6$

$k_{-2} = 0.2640065$

$k_3^0 = 237.1082966$

$\mu = 14.00$

where $k_1[A]$, $k_2[B]$, k_{-1}, k_{-2} and k_3^0 have units $(\sec)^{-1}$.

Then, using (42)-(46) we obtain

$\gamma = 48.00966577$

$\varepsilon = 21.10559431$

$\partial = 2.525190352$

$\varepsilon' = 20.47340573$

$\partial' = 2.059668465$

Since

$$\Delta_\phi = \varepsilon^2 - 4\gamma\partial = -39.48806784 < 0$$

we conclude that ρ_1, ρ_2 are complex.

Using (53), we obtain

$\Psi_1 = 0.2638416181$

$\Psi_1 = 0.1626017947$

Thus, ρ_1, ρ_2 are complex and $0 < \Psi_2 < \Psi_1 < 1$. This is the arrangement (Cal) as shown on page 38.

Using (47), we find that the steady state equation is

$$(237.1082966)y_s^2 e^{-14y_s} + 3.429261841 y_s - 1.262595176 = 0 \quad (110)$$

Since $\beta_2 = 0$ and $\beta_1 \equiv k_{-1}/k_{-2} = 0.631297588$, (12) yields

$$x_s = y_s / \ 0.631297588 \qquad (111)$$

The solution of (110) in (0,1) is ;

$y_s = 0.20$, and using (111) we have $x_s = 0.3168078$.

A sufficient condition for uniqueness for all τ for equation (110) is

$$(1 - \mu\delta)^2 < 4\delta\mu \qquad (109)$$

Using (58), we obtain

$$\delta = 0.3681827853$$

Thus,

$$(1 - \mu\delta)^2 = 17.26036044$$

$$4\mu\delta = 20.61823598$$

Therefore, (109) is satisfied for the values assumed in this example.

According to table 5.11, when ρ_1, ρ_2 are complex and $0 < \Psi_2 < y_s < \Psi_1 < 1$ we have that

$$\Phi(y_s) > 0$$

$$G(y_s) > 0$$

and the steady state is either an unstable focus or an an unstable node.

Using (30)-(33), we obtain

$$\alpha_1 = 0.9053474166$$

$$\alpha_2 = 62.59813151$$

$$\alpha_3 = -39.51804943$$

$$\beta = 4.430673167$$

According to (15)-(16), we have

$$\det \underline{A} = \alpha_1 + e^{-\mu y_s}\left[\alpha_2 y_s + \alpha_3 x_s(\mu y_s - 1)\right]$$

$$tr\underline{A} = -\beta + K_3^{\circ} e^{-\mu y_s}\left[x_s(\mu y_s - 1) - y_s\right]$$

Substituting, we find that

$$\det\underline{A} = 0.2962920094 > 0$$

$$tr\underline{A} = 0.9078607617 > 0$$

Since

$$D = (tr\underline{A})^2 - 4(\det\underline{A}) = -0.3609568729 < 0,$$ then

according to theorem 3.1 the point (0.3168078, 0.20) is an unstable focus.

The characteristic equation for the linearized system is

$$\lambda^2 - (tr\underline{A})\lambda + (\det\underline{A}) = 0$$

The eigenvalues are

$$\lambda_{1,2} = \frac{(tr\underline{A})}{2} \pm \frac{\sqrt{(tr\underline{A})^2 - 4(\det\underline{A})}}{2}$$

For this example,

$$\lambda_1 = 0.4539303809 + i\ (0.3003984325)$$

$$\lambda_2 = 0.4539303809 - i\ (0.3003984325)$$

EXAMPLE 2

This example is related to the previous one. Suppose that

$k_1[A] = k_2[B] = 2.00$

$k_{-1} = 1/6$

$k_{-2} = 0.2640065$

$k_3^0 = 339.3304816$

$\mu = 15.83025413$

where $k_1[A]$, $k_2[B]$, k_{-1}, k_{-2} and k_3^0 have units $(sec)^{-1}$.

Using (42)-(46), we obtain

$\gamma = 54.28608642$

$\varepsilon = 23.41646432$

$\partial = 2.525190352$

$\varepsilon' = 22.78427579$

$\partial' = 2.059668465$

Since

$\Delta\phi = \varepsilon^2 - 4\gamma\partial = -5.2526*10^{-6} < 0$, we conclude that ρ_1, ρ_2 are complex.

Using (53), we obtain

$$\Psi_1 = 0.2879407886$$

$$\Psi_2 = 0.1317666778$$

Thus, ρ_1, ρ_2 are complex and $0 < \Psi_2 < \Psi_1 < 1$. This is the arrangement Ca1 as shown on page 38.

Using (47), we find that the steady state equation is

$$(339.3304816)y_s^2 e^{-15.83025413\, y_s} + 3.429261841 y_s - 1.262595 = 0 \quad (112)$$

We also have that

$$x_s = y_s / 0.631297588 \quad (113)$$

A sufficient condition for uniqueness for all τ for equation (112) is

$$(1 - \mu\delta)^2 < 4\mu\delta \quad (109)$$

Using (58), we obtain

$$\delta = 0.3681827853$$

Thus,

$$(1 - \mu\delta)^2 = 23.31370783$$

$$4\mu\delta = 23.313708823$$

Therefore, (109) is satisfied for the values assumed in this example.

The solution of (112) in the interval (0,1) is

$$y_s = 0.25$$

and using (113)

$$x_s = 0.39600975$$

Since ρ_1, ρ_2 are complex and $0 < \Psi_2 < y_s < \Psi_1 < 1$, we have the arrangement (Ca12). According to table 5.11, for this arrangement

$$\Phi(y_s) > 0$$

$$G(y_s) > 0$$

and the steady state solution is either an unstable focus or an unstable node.

Using (30)-(33) we obtain

$\alpha_1 = 0.9053474166$

$\alpha_2 = 89.58545279$

$\alpha_3 = -56.55508027$

$\beta = 4.430673167$

According to (15)-(16), we have

$$\det\underline{A} = \alpha_1 + e^{-\mu y_s}[\alpha_2 y_s + \alpha_3 x_s(\mu y_s - 1)]$$

$$tr\underline{A} = -\beta + K_3^o e^{-\mu y_s}[x_s(\mu y_s - 1) - y_s]$$

Substituting, we find that

$$\det\underline{A} = 0.0675377564 > 0$$

$$tr\underline{A} = 1.542981473 > 0$$

Since

$$D = (tr\underline{A})^2 - 4(\det\underline{A}) = 2.110640802 > 0 \text{ , then}$$

according to theorem 3.1, the point (0.39600975, 0.25) is an unstable node.

The eigenvalues are

$$\lambda_1 = 1.497892967$$
$$\lambda_2 = 0.0450885062$$

VIIb] Numerical integration of the dynamic equations.

In examples 1 and 2, parameter values were presented for which a unique, unstable steady state solution exists for equation (47). In other words, these values are such that

$$(1 - \mu\delta)^2 < 4\mu\delta$$

and

$$\det\underline{A} > 0$$
$$\operatorname{tr}\underline{A} > 0$$

Here, the dynamic equations

$$\frac{dx}{dt} = K_1[A](1-x-y) - K_{-1}x - K_3^0 e^{-\mu y} xy \qquad (8)$$

$$\frac{dy}{dt} = K_2[B](1-x-y) - K_{-2}y - K_3^0 e^{-\mu y} xy \qquad (9)$$

give rise to limit cycles.

Dividing (9) by (8), we obtain

$$\frac{dy}{dx} = \frac{K_2[B](1-x-y) - K_{-2}y - K_3^0 xy\, e^{-\mu y}}{K_1[A](1-x-y) - K_{-1}x - K_3^0 xy\, e^{-\mu y}} \qquad (114)$$

(114) is a nonlinear, ordinary differential equation which

can be solved numerically. As initial values for $x \in (0,1)$ and $y \in (0,1)$, we can choose values along the sides of a square with corners the points (0,0), (0,1), (1,1) and (1,0).

The numerical integration technique used in this study was a fourth order Runge-Kutta; we employed subroutine RK2, which can be found on page 332 of [18]. The programs were run on the UNIVAC 1108 computer at the University of Houston.

For the parameter values cited in the two examples, equation (114) was numerically integrated with different x and y initial values for each run. The integration was performed with a stepsize 10^{-3}, and the resulting trajectories were plotted in order to examine the phase plane behavior of equations (8)-(9).

In both examples, limit cycling was observed as shown in figures 7.1 and 7.2. By perturbing the unique, unstable steady state, we were able to eliminate the possibility of an unstable limit cycle surrounded by a stable one. The figures show that trajectories originating from the inside give rise to a stable limit cycle.

Figure 7.1 represents example 1, while figure 7.2 corresponds to example 2. The time dependence of x and y for each of these examples can be determined by integrating numerically the dynamic equations (8)-(9). The numerical integration was performed by using subroutine RKGS [18], and the results are shown in figures 7.1a and 7.2a corresponding to examples 1 and 2, respectively. From figure

7.1a we read that the period of oscillations is approximately 11 seconds, while from figure 7.2a we see that it is about 17 seconds.

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IMPORTANT REMARK

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It is essential to emphasize at this point that our region of interest is not the above mentioned square, but actually the orthogonal triangle which has as sides the positive X and Y axes and the line x+y=1. Thus, our search is reduced by a factor of two, because if a limit cycle exists it should definately be restricted in this region.

At this point, it is pertinent to state the following important theorem:

BENDIXSON'S SECOND THEOREM: Consider a two-dimensional system whose state variables are bounded, and which has a unique, unstable steady state. Then all system trajectories are either a stable limit cycle, or else approach a stable limit cycle asymptotically.

A statement of this theorem can be found in:
N. Minorsky, "Nonlinear Oscillations", Ch. 3, Van Nostrand, Princeton, N.J., 1962.

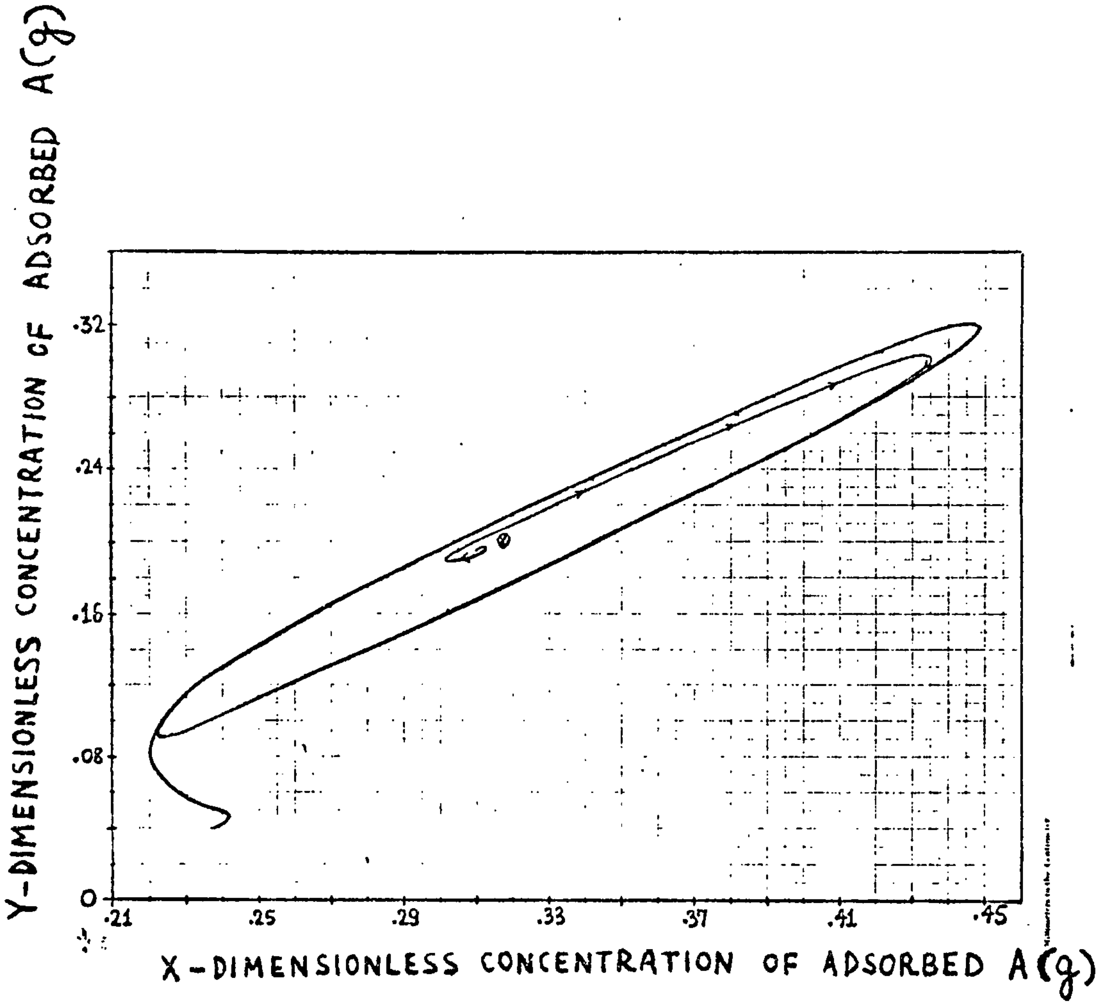

Fig. 7.1. Phase plane trajectories, example 1, μ=14.0

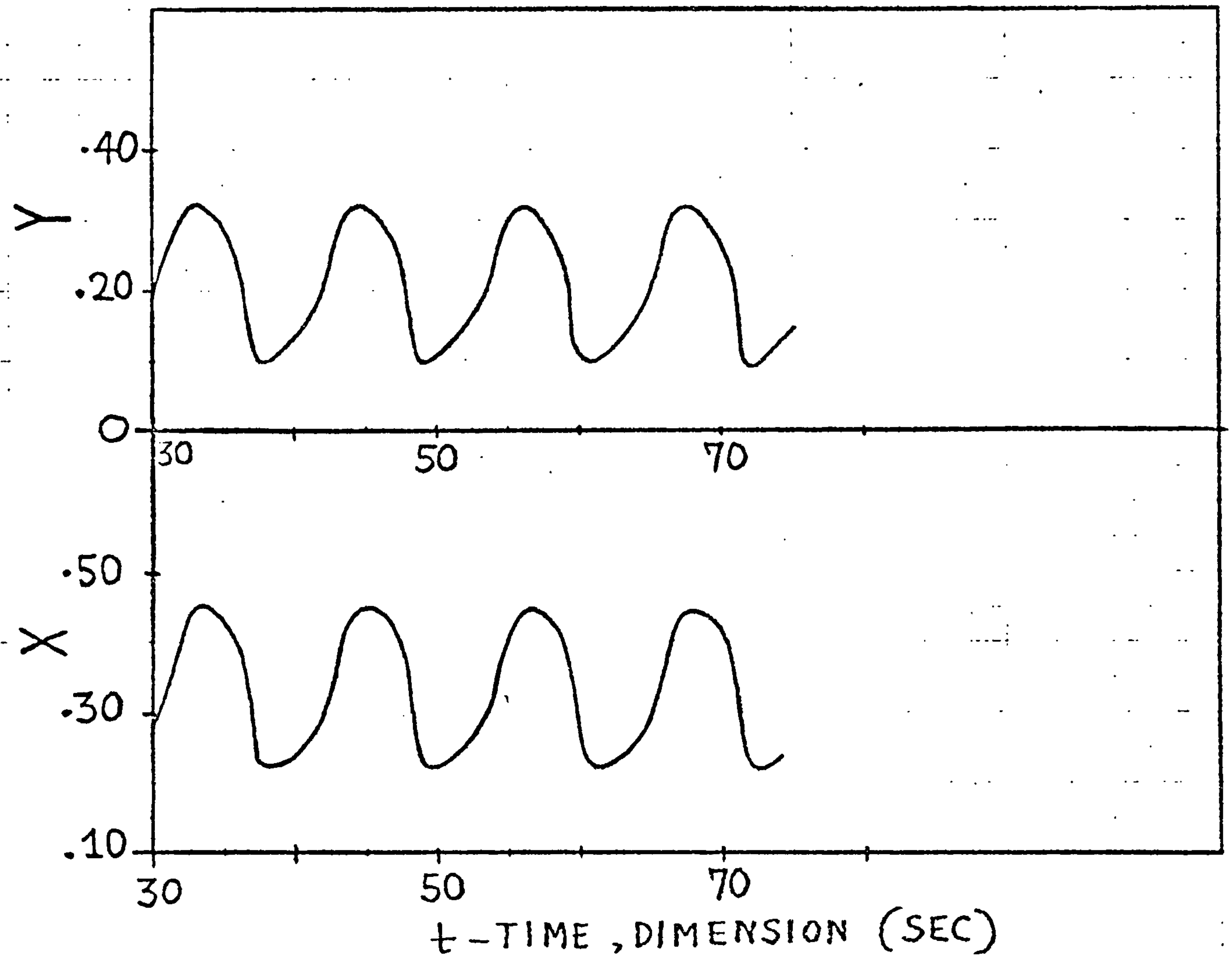

Fig. 7.1a. Dimensionless concentrations of adsorbed reactants versus time, example 1, μ=14.0

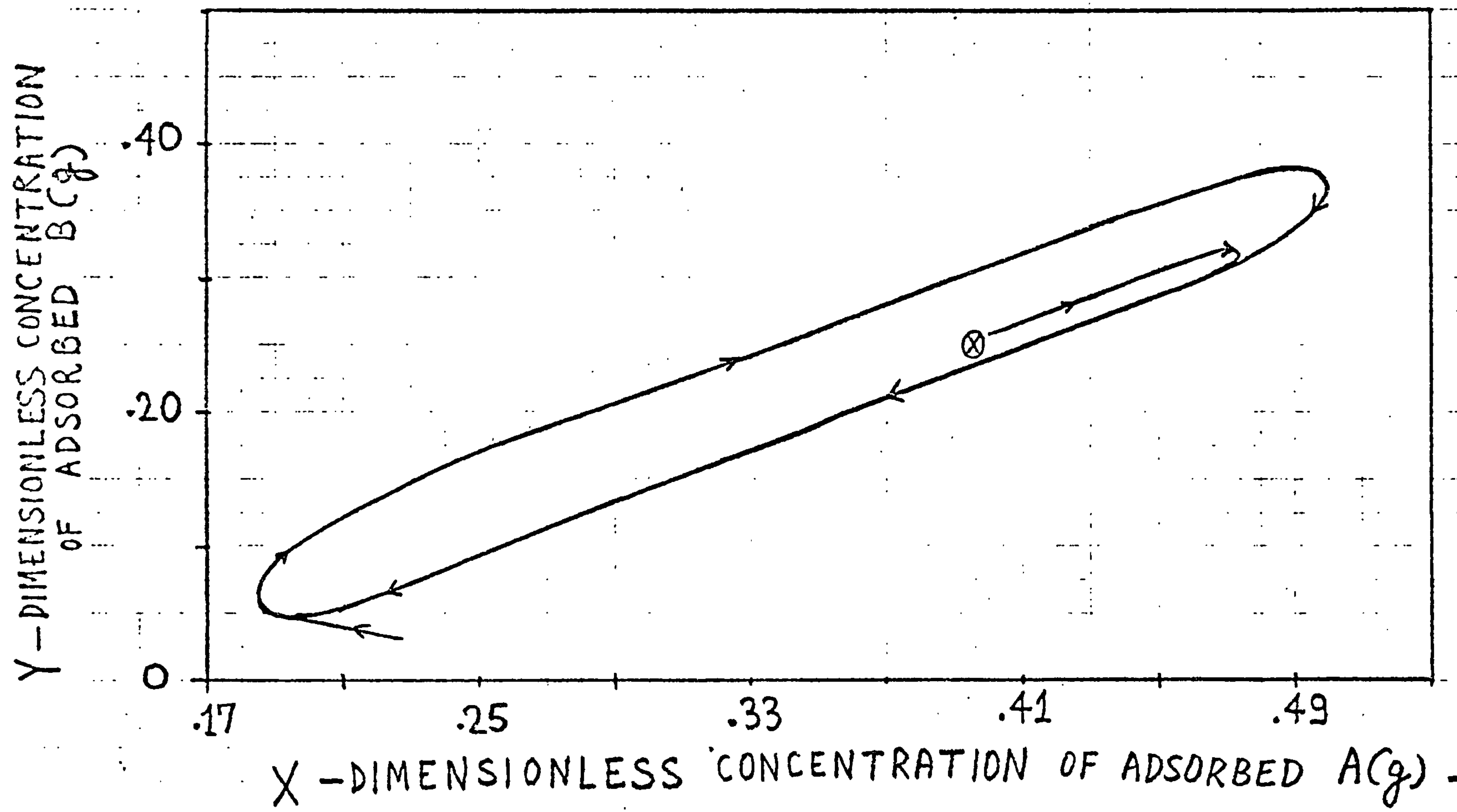

Fig. 7.2. Phase plane trajectories, example 2, μ=15.83025413

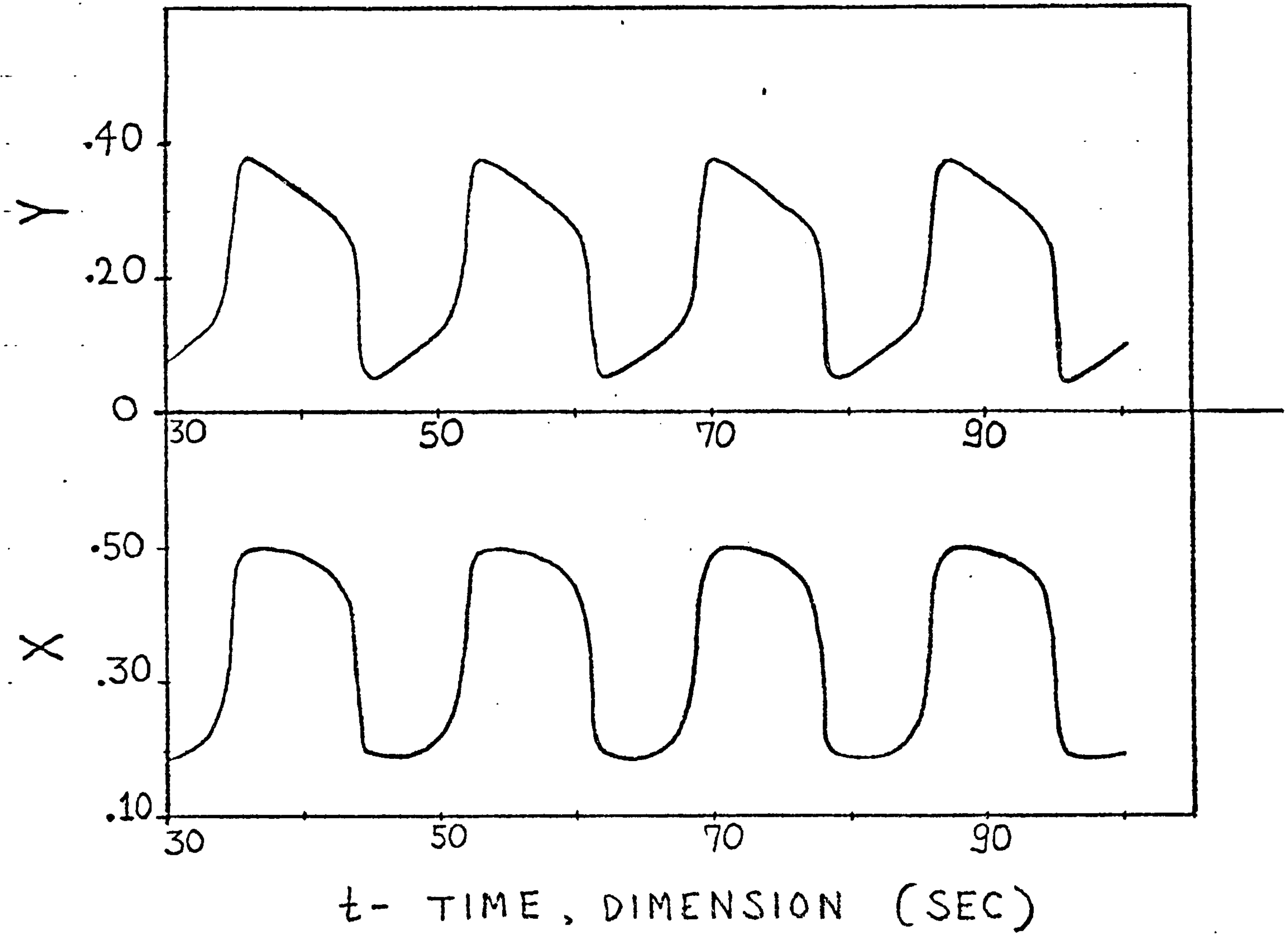

Fig 7.2a. Dimensionless concentrations of adsorbed reactants versus time, example 2, μ=15.83025413

CHAPTER VIII

Here we investigate whether sustained oscillations occur when equ.(47) has multiple steady state solutions. The investigation is carried out by using bifurcation theory.

Multiple steady states and applications of bifurcation theory.

In the previous chapter, we presented examples demonstrating that the dynamic equations can give rise to limit cycles in the case of a unique, unstable steady state solution.

Since we are interested in the phase plane behavior of equs.(8)-(9), we need to investigate whether limit cycles can occur when multiple steady state solutions exist. We will commence our investigation by presenting the following numerical example.

Suppose that

$k_1[A] = k_2[B] = 1.00 \quad (\text{sec})^{-1}$

$k_{-1} = 2.00 \quad (\text{sec})^{-1}$

$k_{-2} = 4.00 \quad (\text{sec})^{-1}$

$k_3^0 = 1604.719045 \quad (\text{sec})^{-1}$

$\mu = 50.00$

Then using (42)-(46) we obtain

$\gamma = 175.00$

$\varepsilon = 28.50$

$\partial = 1.00$

$\varepsilon' = 26.25$

$\partial' = 0.75$

Using (52)-(53) we obtain

$\rho_1 = 0.1116994573$

$\rho_2 = 0.0511576855$

$\Psi_1 = 0.1115962527$

$\Psi_2 = 0.0384037472$

Thus,

$$0 < \Psi_2 < \rho_2 < \Psi_1 < \rho_1 < 1$$

This is the arrangement (Ab1) as shown on page 26.

Using (47), we find that the steady state equation is

$$(1604.719045)\, y_s^2 e^{-50 y_s} + 3.5 y_s - 0.5 = 0 \tag{115}$$

(115) does not satisfy the sufficient condition for uniqueness :

$$(1 - \mu\delta)^2 \leq 4\mu\delta \tag{109}$$

Using (58), we obtain

$$\delta = 1/7$$

Thus,

$$(1 - \mu\delta)^2 = 37.73469$$

$$4\mu\delta = 28.571428$$

Therefore, (109) is not satisfied for the parameter values assumed in this example, and, consequently, equ.(115) has multiple steady states.

Since $\beta_2 = 0$ and $\beta_1 \equiv k_{-1}/k_{-2} = 0.5$, (12) yields

$$x_s = 2y_s \tag{116}$$

Equ.(115) has the following solutions in (0,1) :

$y_{s1} = 0.045$; using (116), $x_{s1} = 0.090$

$y_{s2} = 0.132$, and $x_{s2} = 0.264$

$y_{s3} = 0.058$, and $x_{s3} = 0.116$

Using (30)-(33), we obtain

$\alpha_1 = 14.00$

$\alpha_2 = 6418.87618$

$\alpha_3 = -3209.43809$

$\beta = 8.00$

According to (15)-(16), we have

$$\det \underline{A} = \alpha_1 + \exp(-\mu y_s) * [\alpha_2 y_s + \alpha_3 x_s(\mu y_s - 1)]$$

$$\mathrm{tr}\, \underline{A} = -\beta + K_3^0 \exp(-\mu y_s) * [x_s(\mu y_s - 1) - y_s]$$

Since $0 < \Psi_2 < y_{s1} < \rho_2 < \Psi_1 < \rho_1 < 1$, we have the arrangement (Ab14). According to table 5.2, for this arrangement we have that

$$\Phi(y_{s1}) > 0$$

$$G(y_{s1}) > 0$$

and the steady state is either an unstable focus or an unstable node.

Substituting, we find that for $y_{s1} = 0.045$ and $x_{s1} = 0.09$

$$\det\underline{A} = 6.388873565 > 0$$

$$\mathrm{tr}\underline{A} = 3.416689651 > 0$$

Since

$$D = (\mathrm{tr}\underline{A})^2 - 4(\det\underline{A}) = -13.88172607 < 0,$$ then

according to theorem 3.1 the point (0.090,0.045) is an unstable focus.

Since $0 < \Psi_2 < \rho_2 < \Psi_1 < \rho_1 < y_{s2} < 1$, we have the arrangement (Ab11). According to table 5.2, for this arrangement

$$\Phi(y_{s2}) > 0$$
$$G(y_{s2}) < 0$$

and the steady state is either a stable focus or a stable node.

Substituting, we find that for $y_{s2} = 0.132$ and $x_{s2} = 0.264$

$$\det\underline{A} = 8.697908959 > 0$$
$$\mathrm{tr}\underline{A} = -5.060797358 < 0$$

Since

$D = (\mathrm{tr}\underline{A})^2 - 4(\det\underline{A}) = -9.179965917 < 0$, then according to theorem 3.1 the point (0.264,0.132) is a stable focus.

Since $0 < \Psi_2 < \rho_2 < y_{s3} < \Psi_1 < \rho_1 < 1$, we have the arrangement (Ab13). According to table 5.2, for this arrangement

$$\Phi(y_{s3}) < 0$$
$$G(y_{s3}) > 0$$

and the steady state is a saddle point.

Substituting, we find that for $y_{s3} = 0.058$ and $x_{s3} = 0.116$

$$\det\underline{A} = -4.436373749 < 0$$
$$\mathrm{tr}\underline{A} = 6.339401805 > 0$$

Therefore, the point (0.116,0.058) is a saddle point according to theorem 3.1.

<u>Conclusion :</u> For the parameter values cited in this example, equ.(47) has multiple steady state solutions in the interval (0,1); these solutions are:

$y_{s1} = 0.045$, $x_{s1} = 0.090$: Unstable focus.

$y_{s2} = 0.132$, $x_{s2} = 0.264$: Stable focus.

$y_{s3} = 0.058$, $x_{s3} = 0.116$: Saddle point.

Numerical integration of (114) for the above mentioned parameter values with a stepsize 10^{-3} does not give rise to limit cycles. By using values along the boundaries of the feasible domain as initial values for x and y, we see that all trajectories go to the stable focus; the same is true when we perturb the unstable focus, as shown in figure 8.1. We cannot conclude, however, that limit cycles do not arise for other kinetic parameter values for which (47) has multiple steady state solutions in (0,1).

Thus, we would like to examine whether it is possible to have sustained oscillations in the case of multiple steady state solutions for equ.(47). We will try to solve this problem by using bifurcation theory: We will examine whether limit cycles bifurcate(originate) from critical points, which are centers for the linearized problem associated with the dynamic equations. Poore and coworkers have published in their work [9,10] a large number of examples where bifurcation theory is applied.

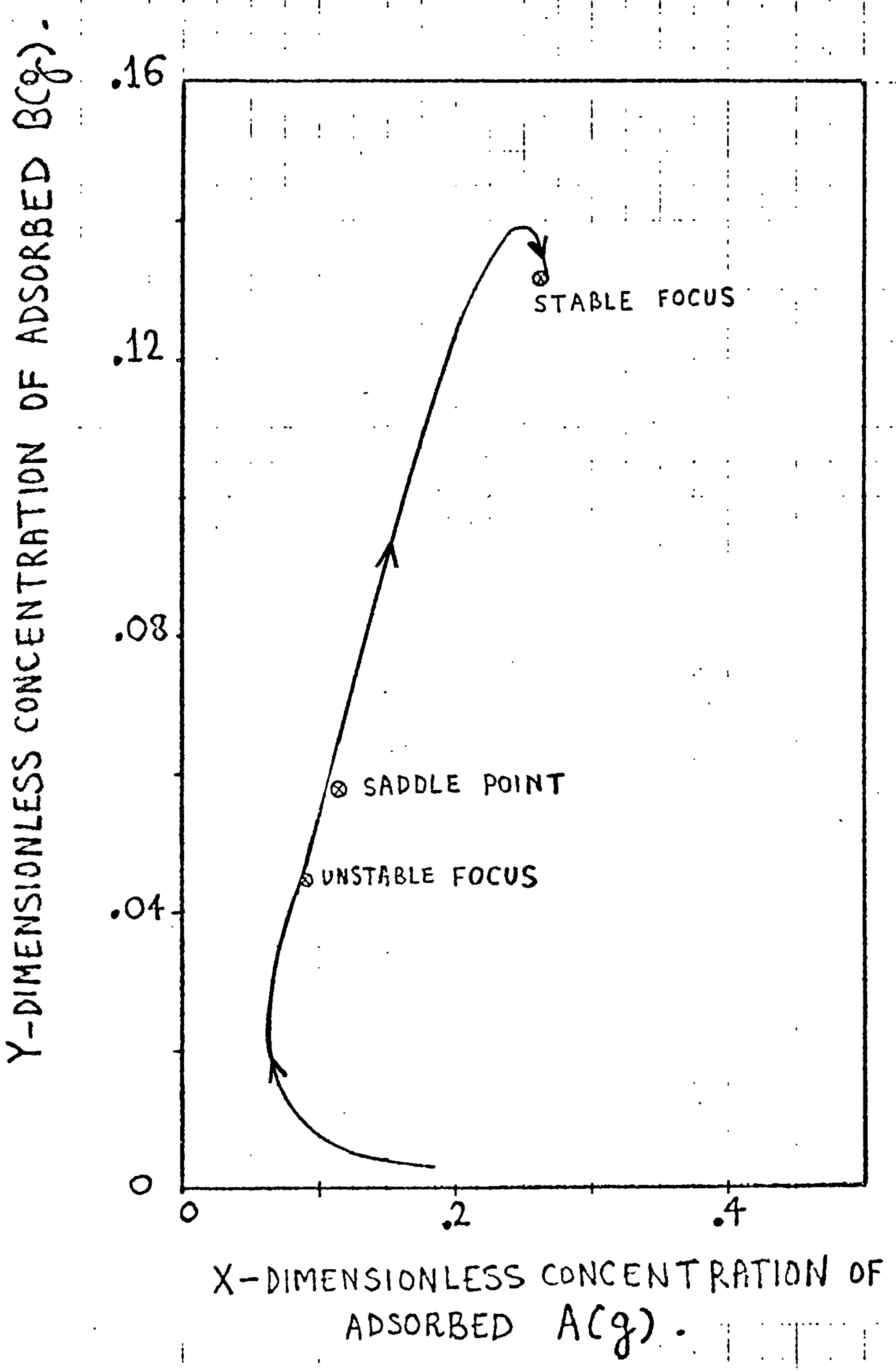

Fig. 8.1. Phase plane trajectories, multiple steady states, μ=50.00

Bifurcation theory is concerned with the variation of a single parameter. In the following example we will vary k_3^0 and let the other five kinetic parameters have the same values as in the previous example; that is, let

$k_1[A] = k_2[B] = 1.00 \quad (sec)^{-1}$

$k_{-1} =-2.00 \quad (sec)^{-1}$

$k_{-2} = 4.00 \quad (sec)^{-1}$

$\mu = 50.00$

Using equ.(47), we find that in this case the steady state equation is

$$k_3^0 y_s^2 e^{-50y_s} + 3.5y_s - 0.5 = 0 \tag{117}$$

Then,

$$k_3^0 = \frac{(0.5-3.5y_s)e^{50y_s}}{y_s^2} \tag{118}$$

Since $k_3^0 > 0$, y_s is restricted in the interval (0,0.1428571429). We can draw a graph of y_s versus k_3^0 , as shown in figure 8.2.

The characteristic equation for the linearized system is

$$\lambda^2 - (\mathrm{tr}\underline{A})\lambda + (\det\underline{A}) = 0$$

The eigenvalues are

$$\lambda_{1,2} = \frac{(\mathrm{tr}\underline{A})}{2} \pm \frac{\sqrt{(\mathrm{tr}\underline{A})^2 - 4(\det\underline{A})}}{2}$$

Bifurcation of periodic solutions can occur only from the center or possibly at those points at which one of the eigenvalues of $\underline{A}$ is equal to zero [9]. According to theorem

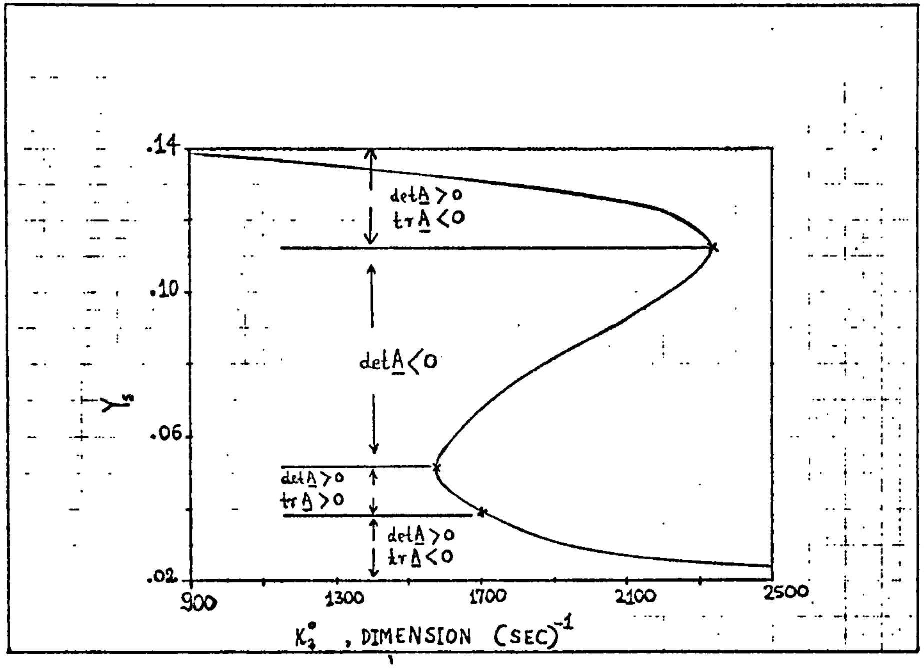

Fig. 8.2. Locus of system steady states.

3.1, the critical point (x_s, y_s) will be a center for the linearized problem if the eigenvalues of $\underline{A}$ are purely imaginary:

$$\mathrm{tr}\underline{A} = 0 \quad \text{and } \det\underline{A} > 0$$

For the parameter values cited in this section, the center is

$$y_s = \Psi_2 = 0.0384037472, \; x_s = 0.0768074944$$

Using (118), we find that at the center $k_3^0 = 1691.103454$. Thus, we are able to locate the center for the linearized problem on the y_s versus k_3^0 graph (fig. 8.2). By increasing the value of k_3^0 above its value at the center, and integrating numerically the ordinary differential equation

$$\frac{dy}{dx} = \frac{K_2[B](1-x-y) - K_{-2}y - K_3^0 xy\, e^{-\mu y}}{K_1[A](1-x-y) - K_{-1}x - K_3^0 xy\, e^{-\mu y}} \tag{114}$$

we find that there are no limit cycles in the phase plane; the same is true when we integrate (114) for values of k_3^0 which are smaller than its value at the center. The numerical integrations were carried-out with a stepsize 10^{-3}.

Therefore, we can draw the conclusion that this particular set of kinetic parameters does not give rise to limit cycles. It is possible, however, that there are other parameters for which sustained oscillations may exist in the case of multiple steady state solutions.

CHAPTER IX

Conclusions

In this study, we have attempted to investigate the stability characteristics of a surface kinetics mechanism representing a general chemical reaction. Our main objective was to examine the validity of statements made by Slinko and coworkers [5] concerning the observance of concentration oscillations during the isothermal oxidation of hydrogen on a nickel foil.

Because we wanted to keep the mathematical analysis as simple as possible, rather than working on a specific chemical reaction we prefered to analyze the general reaction $A(g) + B(g) \longrightarrow AB$. We assumed that the heterogeneous catalytic mechanism for this reaction is a Langmuir-Hinshelwood type, and the adsorbed B(g) changes the properties of the catalytic surface such that the energy of activation for the surface reaction depends linearly on the coverage by adsorbed B(g).

We derived the differential equations for the net rates of adsorption of A(g) and B(g), and linearized them about the steady state in order to investigate the local stability characteristics of the critical points, by using the first method of Liapunov. Expressions were derived for the determinant and trace of the linearized matrix $\underline{A}$, and for simplicity we decided to assume in our stability analysis that $k_1[A] = k_2[B]$.

The nature of the critical points depends on the sign of det$\underline{A}$ and tr$\underline{A}$. We have been able to derive, however, the polynomials $\Phi(y_s)$ and $G(y_s)$ having the same sign as det$\underline{A}$ and tr$\underline{A}$. The signs of $\Phi(y_s)$ and $G(y_s)$ depend on the size of the critical point with respect to the relative positions of the roots of the equations $\Phi(\xi) = 0$, $G(\omega) = 0$, in the interval (0,1). We have also been able to derive the necessary and sufficient conditions for all possible arrangements of the root positions for the equations $\Phi(\xi) = 0$, $G(\omega) = 0$, in (0,1).

Uniqueness criteria were developed for the steady state solutions both for the general case and when $k_1[A] = k_2[B]$. Using these uniqueness criteria and the necessary and sufficient conditions for the arrangement of the root positions for the equations $\Phi(\xi) = 0$, $G(\omega) = 0$ in the interval (0,1), we were able to find parameter values for which the dynamic equations give rise to limit cycles. These limit cycles were found for the case of a unique, unstable steady state solution.

We used principles of bifurcation theory to investigate the existence of sustained oscillations for the case of multiple steady states. By varying one of the kinetic parameters and numerically integrating the dynamic equations, we checked whether periodic orbits bifurcate(originate) from critical points which are centers for the linearized problem. Our efforts have led us to conclude that limit cycles do not exist for the kinetic parameter values chosen in that particular example. It is possible, however, that there are other values for which sustained oscillations could be observed in the case of multiple steady state solutions; this is, of course, only an assumption and will have to be proved.

Slinko and coworkers [5] do not give in their paper any kinetic parameter values, or show numerical simulations to demonstrate that their proposed kinetic mechanism gives rise to limit cycles such that is in agreement with experimental results. Our study has shown that there are parameter values for which sustained oscillations arise in the case of a unique, unstable steady state. Our kinetic mechanism, although simpler than Slinko's, does have similar features and is based on the same assumptions.

In our study, the stability analysis was performed for the special case $k_1[A] = k_2[B]$. It would be rather interesting, however, to investigate the general case $k_1[A] \neq k_2[B]$, in order to get a picture of the phase plane behavior of the dynamic equations.

It is possible that the chemical reaction proceeds by an Eley-Rideal rather than a Langmuir-Hinshelwood kinetic mechanism. Then it would be interesting to assume that the reaction has features belonging to both possible kinetic mechanisms. An even more difficult problem to consider is one where we take into account diffusional limitations and mass tranfer resistance such as in the case of a catalytic pellet.

APPENDIX

Section 1

Consider the polynomials

$$\Phi(y_s)=\gamma y_s^2-\varepsilon y_s+\vartheta \tag{40}$$

$$G(y_s)=-\gamma y_s^2+\varepsilon' y_s-\vartheta' \tag{41}$$

then, we can state the following theorems [20] :

Theorem A1 : Suppose that the polynomial $\Phi(y_s)$ has real and unequal roots $\rho_1>\rho_2$. Then, the necessary and sufficient conditions for $m<\rho_2<\rho_1$ are:

$$\Delta_\phi>0,\ \gamma\Phi(m)>0,\ m<\frac{\rho_1+\rho_2}{2}$$

where m is a real number.

Theorem A2 : Suppose that the polynomial $G(y_s)$ has real and unequal roots $\psi_1>\psi_2$. Then, the necessary and sufficient conditions for $m<\psi_2<\psi_1$ are:

$$\Delta_G>0,\ -\gamma G(m)>0,\ m<\frac{\psi_1+\psi_2}{2},$$

where m is a real number.

Theorem A3 : Suppose that the polynomial $\Phi(y_s)$ has real and unequal roots, $\rho_1>\rho_2$. Then, the necessary and sufficient conditions for $\rho_2<\rho_1<M$ are:

$$\Delta_\phi>0,\ \gamma\Phi(M)>0,\ M>\frac{\rho_1+\rho_2}{2},$$

where M is a real number.

Theorem A4 : Suppose that the polynomial $G(y_s)$ has real and unequal roots $\psi_1 > \psi_2$. Then, the necessary and sufficient conditions for $\psi_2 < \psi_1 < M$ are:

$$\Delta_G > 0, \; -\gamma G(M) > 0, \; M > \frac{\psi_1 + \psi_2}{2}$$

where M is a real number.

Theorem A5 : Suppose that $\rho_2 < \eta < \rho_1$, where ρ_1, ρ_2 are roots of the polynomial $\Phi(y_s)$; then, we have that $\gamma \Phi(\eta) < 0$. The reverse is also true: If η is a real number and $\gamma \Phi(\eta) < 0$, then the roots of $\Phi(y_s)$ are real and unequal and η lies between the roots.

Theorem A6 : Suppose that $\psi_2 < \eta < \psi_1$, where ψ_1, ψ_2 are roots of the polynomial $G(y_s)$; then, we have that $-\gamma G(\eta) < 0$. The reverse is also true: If η is a real number and $-\gamma G(\eta) < 0$, then the roots of $G(y_s)$ are real and unequal and η lies between the roots.

Section 2

Suppose that we have the polynomials

$$\Phi(y_s) = \gamma y_s^2 - \varepsilon y_s + \vartheta \tag{40}$$

$$G(y_s) = -\gamma y_s^2 + \varepsilon' y_s - \vartheta' \tag{41}$$

where ρ_1, ρ_2 are the roots of $\Phi(\xi) = 0$, and ψ_1, ψ_2 are the roots of $G(\omega) = 0$. Then, the following relations exist :

$$\rho_1 + \rho_2 = \varepsilon/\gamma \tag{A1}$$

$$\rho_1 \rho_2 = \vartheta/\gamma \tag{A2}$$

$$\psi_1 + \psi_2 = \varepsilon'/\gamma \tag{A3}$$

$$\psi_1 \psi_2 = \vartheta'/\gamma \tag{A4}$$

$$\rho_1^2 + \rho_2^2 = (\varepsilon^2 - 2\gamma\vartheta)/\gamma^2 \tag{A5}$$

$$\psi_1^2 + \psi_2^2 = (\varepsilon'^2 - 2\gamma\vartheta')/\gamma^2 \tag{A6}$$

$$\gamma\{\Phi(\psi_1) + \Phi(\psi_2)\} = \varepsilon'^2 - \varepsilon\varepsilon' + 2\gamma(\vartheta - \vartheta') \tag{A7}$$

$$-\gamma\{\mathcal{G}(\rho_1) + \mathcal{G}(\rho_2)\} = \varepsilon^2 - \varepsilon\varepsilon' - 2\gamma(\vartheta - \vartheta') \tag{A8}$$

$$R_{\mathcal{G}\phi} = \gamma^2\Phi(\psi_1)\Phi(\psi_2) = \gamma^2\mathcal{G}(\rho_1)\mathcal{G}(\rho_2) = \gamma^2(\vartheta' - \vartheta)^2 - \gamma(\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta') \tag{A9}$$

$$\gamma\Phi(0) = \gamma\vartheta \tag{A10}$$

$$\gamma\Phi(1) = \gamma(\gamma - \varepsilon + \vartheta) \tag{A11}$$

$$-\gamma\mathcal{G}(0) = \gamma\vartheta' \tag{A12}$$

$$-\gamma\mathcal{G}(1) = \gamma(\gamma - \varepsilon' + \vartheta') \tag{A13}$$

$$-\gamma\mathcal{G}(\varepsilon/2\gamma) = \gamma\vartheta' + \frac{\varepsilon}{2}\left(\frac{\varepsilon}{2} - \varepsilon'\right) \tag{A14}$$

$$\gamma\Phi(\varepsilon'/2\gamma) = \gamma\vartheta + \frac{\varepsilon'}{2}\left(\frac{\varepsilon'}{2} - \varepsilon\right) \tag{A15}$$

Section 3

Consider the polynomials

$$\Phi(y_s)=\gamma y_s^2-\varepsilon y_s+\vartheta \tag{40}$$

$$G(y_s)=-\gamma y_s^2+\varepsilon' y_s-\vartheta' \tag{41}$$

which have no common roots. Let ρ_1, ρ_2 be the roots of $\Phi(\xi)=0$, and ψ_1, ψ_2 be the roots of $G(\omega)=0$. Then, we state the following theorem [20] :

Theorem A7 : Suppose that ρ_1, ρ_2 are real and unequal, $\rho_1 > \rho_2$; similarly, that ψ_1, ψ_2 are real and unequal, $\psi_1 > \psi_2$. Then,. we can distinguish the following subcases :

a] $\rho_2 < \psi_2 < \rho_1 < \psi_1$

The necessary and sufficient conditions for this arrangement are

$$R_{G\phi} < 0 \tag{A16}$$

$$\rho_1+\rho_2 < \psi_1+\psi_2 \tag{A17}$$

b] $\psi_2 < \rho_2 < \psi_1 < \rho_1$

The necessary and sufficient conditions for this arrangement are

$$R_{G\phi} < 0 \tag{A18}$$

$$\psi_1+\psi_2 < \rho_1+\rho_2 \tag{A19}$$

c] $\rho_2 < \psi_2 < \psi_1 < \rho_1$

The necessary and sufficient conditions for this arrrangement are

$$\Delta_G > 0 \tag{A20}$$

$$R_{G\phi} > 0 \tag{A21}$$

$$\gamma\{\Phi(\Psi_1)+\Phi(\Psi_2)\} < 0 \tag{A22}$$

d] $\Psi_2 < \rho_2 < \rho_1 < \Psi_1$

The necessary and sufficient conditions for this arrangement are

$$\Delta_\phi > 0 \tag{A23}$$

$$R_{G\phi} > 0 \tag{A24}$$

$$-\gamma\{G(\rho_1)+G(\rho_2)\} < 0 \tag{A25}$$

e] $\rho_2 < \rho_1 < \Psi_2 < \Psi_1$

The necessary and sufficient conditions for this arrangement are

$$\Delta_\phi > 0 \tag{A26}$$

$$\Delta_G > 0 \tag{A27}$$

$$R_{G\phi} > 0 \tag{A28}$$

$$\gamma\{\Phi(\Psi_1)+\Phi(\Psi_2)\} > 0 \tag{A29}$$

$$-\gamma\{G(\rho_1)+G(\rho_2)\} > 0 \tag{A30}$$

$$\rho_1+\rho_2 < \Psi_1+\Psi_2 \tag{A31}$$

f] $\Psi_2 < \Psi_1 < \rho_2 < \rho_1$

The necessary and sufficient conditions for this arrangement are

$$\Delta_{\phi} > 0 \tag{A32}$$

$$\Delta_{G} > 0 \tag{A33}$$

$$R_{G\phi} > 0 \tag{A34}$$

$$\gamma\{\phi(\psi_1)+\phi(\psi_2)\} > 0 \tag{A35}$$

$$-\gamma\{G(\rho_1)+G(\rho_2)\} > 0 \tag{A36}$$

$$\psi_1+\psi_2 < \rho_1+\rho_2 \tag{A37}$$

Section 4

We can now use theorems (A1)-(A7) to derive the necessary and sufficient conditions for all possible arrangements for the root positions shown in chapter IVb.

CASE A

a1] $0 < \rho_2 < \psi_2 < \rho_1 < \psi_1 < 1$

For the arrangement

$$\rho_2 < \psi_2 < \rho_1 < \psi_1$$

we have from theorem A7a that the necessary and sufficient conditions are (A16)-(A17). Using relations (A9), (A1), and (A3), we can write (A16)-(A17) in the form

$$\gamma(\vartheta'-\vartheta)^2 < (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta') \tag{A38}$$

$$\varepsilon < \varepsilon' \tag{A39}$$

The necessary and sufficient conditions for zero to be smaller than ρ_1, ρ_2, are according to theorem A1 :

$$\Delta_\phi > 0 \quad , \quad \gamma\Phi(0) > 0 \quad , \quad 0 < \frac{\rho_1+\rho_2}{2}$$

Using (A10), (A1), we can write these conditions as

$$\varepsilon^2 - 4\gamma\vartheta > 0 \tag{A40}$$

$$\gamma\vartheta > 0 \tag{A41}$$

$$\varepsilon/2\gamma > 0 \tag{A42}$$

Since γ, ϑ, and ε are all positive by definition, it is obvious that (A41) and (A42) are automatically satisfied. Condition (A40) is actually repetitive, because (A38) guarantees that the roots ρ_1, ρ_2 are real and unequal; therefore, we do not have to require that (A40)-(A42) be satisfied.

According to theorem A4, the necessary and sufficient conditions for 1 to be greater than Ψ_1, Ψ_2 are

$$\Delta_G > 0 \quad , \quad -\gamma G(1) > 0 \quad , \quad 1 > \frac{\Psi_1+\Psi_2}{2}$$

Using (A13), (A3), we can write these conditions as

$$\varepsilon'^2 - 4\gamma\vartheta' > 0 \tag{A43}$$

$$(\gamma - \varepsilon' + \vartheta') > 0 \tag{A44}$$

$$1 > \varepsilon'/2\gamma \tag{A45}$$

However, since (A38) guarantees that ρ_1, ρ_2 are real and unequal and we have the arrangement $\rho_2 < \Psi_2 < \rho_1 < \Psi_1$, it is obvious that ψ_1, ψ_2 will also be real and unequal; therefore, we do not need to include (A43).

In summary, the necessary and sufficient conditions for the arrangement

$$0 < \rho_2 < \psi_2 < \rho_1 < \psi_1 < 1$$

are :

$$\gamma(\vartheta' - \vartheta)^2 < (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta') \tag{A38}$$

$$\varepsilon < \varepsilon' \tag{A39}$$

$$(\gamma - \varepsilon' + \vartheta') > 0 \tag{A44}$$

$$2\gamma > \varepsilon' \tag{A45}$$

Or in a more compact form,

$$\begin{gathered} \gamma(\vartheta' - \vartheta)^2 < (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta') \\ (\gamma - \varepsilon' + \vartheta') > 0 \\ 2\gamma > \varepsilon' > \varepsilon \end{gathered}$$

a2] $0 < \rho_2 < \psi_2 < \rho_1 < 1 < \psi_1$

The necessary and sufficient conditions for the arrangement

$$0 < \rho_2 < \psi_2 < \rho_1 < \psi_1$$

are as before

$$\gamma(\vartheta' - \vartheta)^2 < (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta') \tag{A38}$$

$$\varepsilon < \varepsilon' \tag{A39}$$

The necessary and sufficient conditions for 1 to be between ψ_1 and ψ_2 are according to theorem A6

$$-\gamma G(1) < 0$$

Using (A13), we can write this condition as

$$\gamma(\gamma-\varepsilon'+\vartheta')<0$$

and since $\gamma>0$,

$$(\gamma-\varepsilon'+\vartheta')<0 \qquad \text{(A46)}$$

The necessary and sufficient conditions for 1 to be greater than ρ_1 , ρ_2 , are according to theorem A3

$$\Delta_\phi>0\ ,\ \gamma\phi(1)>0\ ,\ 1>\frac{\rho_1+\rho_2}{2}$$

Using (A11), (A1), we can write these conditions as

$$\varepsilon^2-4\gamma\vartheta>0 \qquad \text{(A47)}$$

$$(\gamma-\varepsilon+\vartheta)>0 \qquad \text{(A48)}$$

$$1>\varepsilon/2\gamma \qquad \text{(A49)}$$

Since (A47) is repetitive, we end-up with the conditions

$$\gamma(\vartheta'-\vartheta)^2<(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta') \qquad \text{(A38)}$$

$$\varepsilon<\varepsilon' \qquad \text{(A39)}$$

$$(\gamma-\varepsilon'+\vartheta')<0 \qquad \text{(A46)}$$

$$(\gamma-\varepsilon+\vartheta)>0 \qquad \text{(A48)}$$

$$2\gamma>\varepsilon \qquad \text{(A49)}$$

Or in a more compact form,

$$\gamma(\vartheta'-\vartheta)^2<(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$

$$\varepsilon<\inf(\varepsilon',2\gamma)$$

$$(\varepsilon-\vartheta)<\gamma<(\varepsilon'-\vartheta')$$

a3] $0<\rho_2<\psi_2<1<\rho_1<\psi_1$

The necessary and sufficient conditions for 1 to be between ψ_1, ψ_2 and between ρ_1, ρ_2 are according to theorems A6, A5,

$$-\gamma G(1)<0$$

$$\gamma \Phi(1)<0$$

Using (A13), (A11), we can write these conditions as

$$\gamma(\gamma-\varepsilon'+\vartheta')<0 \qquad \text{(A50)}$$

$$\gamma(\gamma-\varepsilon+\vartheta)<0 \qquad \text{(A51)}$$

Since $\gamma>0$, we can rewrite these as

$$(\gamma-\varepsilon'+\vartheta'<0 \qquad \text{(A52)}$$

$$(\gamma-\varepsilon+\vartheta)<0 \qquad \text{(A53)}$$

For the arrangement

$$0<\rho_2<\psi_2<\rho_1<\psi_1$$

we have again that the necessary and sufficient conditions are

$$\gamma(\vartheta'-\vartheta)^2<(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta') \qquad \text{(A38)}$$

$$\varepsilon<\varepsilon' \qquad \text{(A39)}$$

In summary, we have that the necessary and sufficient conditions for the arrangement $0<\rho_2<\psi_2<1<\rho_1<\psi_1$ are

$$\gamma(\vartheta'-\vartheta)^2 < (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta') \qquad (A38)$$

$$\varepsilon < \varepsilon' \qquad (A39)$$

$$(\gamma-\varepsilon'+\vartheta') < 0 \qquad (A52)$$

$$(\gamma-\varepsilon+\vartheta) < 0 \qquad (A53)$$

Or in a more compact form,

$$\gamma(\vartheta'-\vartheta)^2 < (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon' > \varepsilon$$
$$\gamma < \inf\{(\varepsilon'-\vartheta'),(\varepsilon-\vartheta)\}$$

a4] $0 < \rho_2 < 1 < \psi_2 < \rho_1 < \psi_1$

The necessary and sufficient conditions for 1 to be less than ψ_1, ψ_2, are according to theorem A2

$$-\gamma G(1) > 0 \quad , \quad 1 < (\psi_1+\psi_2)/2$$

Using (A13), (A3), we write these conditions as

$$\gamma(\gamma-\varepsilon'+\vartheta') > 0 \qquad (A54)$$

$$1 < \varepsilon'/2\gamma \qquad (A55)$$

Since $\gamma > 0$, we can rewrite (A54) as

$$(\gamma-\varepsilon'+\vartheta') > 0 \qquad (A56)$$

$$2\gamma < \varepsilon' \qquad (A55)$$

The necessary and sufficient conditions for 1 to be between ρ_1, ρ_2 are according to theorem A5,

$$\gamma\Phi(1) < 0$$

Using (All), this condition can be written as

$$(\gamma-\varepsilon+\vartheta)<0 \tag{A57}$$

As before, the necessary and sufficient conditions are

$$\gamma(\vartheta'-\vartheta)^2<(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta') \tag{A38}$$

$$\varepsilon<\varepsilon' \tag{A39}$$

In summary, the necessary and sufficient conditions for the arrangement $0<\rho_2<1<\psi_2<\rho_1<\psi_1$ are

$$\gamma(\vartheta'-\vartheta)^2<(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon<\varepsilon'$$
$$(\gamma-\varepsilon'+\vartheta')>0$$
$$2\gamma<\varepsilon'$$
$$(\gamma-\varepsilon+\vartheta)<0$$

Or in a more compact form,

$$\gamma(\vartheta'-\vartheta)^2<(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon'>\sup(\varepsilon,2\gamma)$$
$$(\varepsilon'-\vartheta')<\gamma<(\varepsilon-\vartheta)$$

a5] $1<\rho_2<\psi_2<\rho_1<\psi_1$

The necessary and sufficient conditions for 1 to be less than ρ_1,ρ_2 are according to theorem A1,

$$\gamma\Phi(1)>0 \quad , \quad 1<(\rho_1+\rho_2)/2$$

Using (All), (A1), we can write these conditions as

$$(\gamma-\varepsilon+\vartheta)>0 \tag{A58}$$

$$1 < \varepsilon/2\gamma \qquad \text{(A59)}$$

As before, the necessary and sufficient conditions for the arrangement $\rho_2 < \psi_2 < \rho_1 < \psi_1$ are

$$\gamma(\vartheta' - \vartheta)^2 < (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta') \qquad \text{(A38)}$$

$$\varepsilon < \varepsilon' \qquad \text{(A39)}$$

In summary, the necessary and sufficient conditions for $1 < \rho_2 < \psi_2 < \rho_1 < \psi_1$ are

$$\gamma(\vartheta' - \vartheta)^2 < (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta')$$

$$2\gamma < \varepsilon < \varepsilon'$$

$$(\gamma - \varepsilon + \vartheta) > 0$$

b1] $0 < \psi_2 < \rho_2 < \psi_1 < \rho_1 < 1$

For the arrangement $\psi_2 < \rho_2 < \psi_1 < \rho_1$ we have from theorem A7b that the necessary and sufficient conditions are

$$R_{G\phi} < 0 \quad , \quad \psi_1 + \psi_2 < \rho_1 + \rho_2$$

Using (A9), (A1), (A3), we can write these conditions as

$$\gamma(\vartheta' - \vartheta)^2 < (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta') \qquad \text{(A38)}$$

$$\varepsilon' < \varepsilon$$

The necessary and sufficient conditions for zero to be less than ψ_1, ψ_2 are according to theorem A2

$$-\gamma G(0) > 0 \quad , \quad 0 < (\psi_1 + \psi_2)/2$$

Using (A12), (A3), we can write these conditions as

$$\gamma\vartheta' > 0$$
$$\varepsilon'/2\gamma > 0$$

Since $\gamma, \vartheta', \varepsilon'$ are all positive by definition, it is obvious that both these conditions are automatically satisfied.

The necessary and sufficient conditions for 1 to be greater than ρ_1, ρ_2 are according to theorem A3

$$\gamma\phi(1) > 0 \quad , \quad 1 > (\rho_1+\rho_2)/2$$

Using (A11), (A1), we can write these conditions as

$$(\gamma-\varepsilon+\vartheta) > 0 \qquad \text{(A60)}$$

$$1 > \varepsilon/2\gamma \qquad \text{(A61)}$$

In summary, the necessary and sufficient conditions for the arrangement $0<\psi_2<\rho_2<\psi_1<\rho_1<1$ are

$$\gamma(\vartheta'-\vartheta)^2 < (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon' < \varepsilon$$
$$(\gamma-\varepsilon+\vartheta) > 0$$
$$2\gamma > \varepsilon$$

Or in a more compact form,

$$\gamma(\vartheta'-\vartheta)^2 < (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$(\gamma-\varepsilon+\vartheta) > 0$$
$$\varepsilon' < \varepsilon < 2\gamma$$

b2] $0<\psi_2<\rho_2<\psi_1<1<\rho_1$

The necessary and sufficient conditions for 1 to be between ρ_1, ρ_2 are according to theorem A5

$$\gamma\phi(1) < 0$$

Using (A11),

$$(\gamma-\varepsilon+\vartheta) < 0 \qquad \text{(A62)}$$

The necessary and sufficient conditions for 1 to be greater than ψ_1, ψ_2 are according to theorem A4,

$$-\gamma G(1) > 0 \quad , \quad 1 > (\psi_1 + \psi_2)/2$$

Using (A13), (A3), we can write these conditions as

$$(\gamma - \varepsilon' + \vartheta') > 0 \qquad \text{(A63)}$$

$$1 > \varepsilon'/2\gamma \qquad \text{(A64)}$$

The necessary and sufficient conditions for the arrangement $0 < \psi_2 < \rho_2 < \psi_1 < \rho_1$ are as before,

$$\gamma(\vartheta' - \vartheta)^2 < (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta') \qquad \text{(A38)}$$
$$\varepsilon' < \varepsilon$$

In summary, the necessary and sufficient conditions for the arrangement $0 < \psi_2 < \rho_2 < \psi_1 < 1 < \rho_1$ are

$$\gamma(\vartheta' - \vartheta)^2 < (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta')$$
$$\varepsilon' < \varepsilon$$
$$(\gamma - \varepsilon + \vartheta) < 0$$
$$(\gamma - \varepsilon' + \vartheta') > 0$$
$$2\gamma > \varepsilon'$$

Or in a more compact form,

$$\gamma(\vartheta' - \vartheta)^2 < (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta')$$
$$\varepsilon' < \inf(\varepsilon, 2\gamma)$$
$$(\varepsilon' - \vartheta') < \gamma < (\varepsilon - \vartheta)$$

b3] $0 < \psi_2 < \rho_2 < 1 < \psi_1 < \rho_1$

The necessary and sufficient conditions for 1 to be between ρ_1, ρ_2 and ψ_1, ψ_2 are according to theorems A5 and A6,

$\gamma\Phi(1) < 0$

$-\gamma G(1) < 0$

Using (A11), (A13), we can write these conditions as

$$(\gamma - \varepsilon + \vartheta) < 0 \qquad \text{(A65)}$$

$$(\gamma - \varepsilon' + \vartheta') < 0 \qquad \text{(A66)}$$

The necessary and sufficient conditions for the arrangement $0 < \psi_2 < \rho_2 < \psi_1 < \rho_1$ are as before,

$$\gamma(\vartheta' - \vartheta)^2 < (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta')$$
$$\varepsilon' < \varepsilon$$

In summary, the necessary and sufficient conditions for the arrangement $0 < \psi_2 < \rho_2 < 1 < \psi_1 < \rho_1$ are

$\gamma(\vartheta' - \vartheta)^2 < (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta')$

$\varepsilon' < \varepsilon$

$(\gamma - \varepsilon + \vartheta) < 0$

$(\gamma - \varepsilon' + \vartheta') < 0$

Or in a more compact form,

$$\gamma(\vartheta' - \vartheta)^2 < (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta')$$
$$\varepsilon' < \varepsilon$$
$$\gamma < \inf\{(\varepsilon - \vartheta), (\varepsilon' - \vartheta')\}$$

b4] $0 < \psi_2 < 1 < \rho_2 < \psi_1 < \rho_1$

The necessary and sufficient conditions for 1 to be between ψ_1, ψ_2 are according to theorem A6,

$$-\gamma G(1) < 0$$

Using (A13), we can write this condition as

$$(\gamma - \varepsilon' + \vartheta') < 0 \qquad \text{(A67)}$$

The necessary and sufficient conditions for 1 to be less than ρ_1, ρ_2 are according to theorem A1,

$$\gamma\Phi(1) > 0 \quad , \quad 1 < (\rho_1+\rho_2)/2$$

Using (A11), (A1), we can write these conditions as

$$(\gamma-\varepsilon+\vartheta) > 0 \qquad \text{(A68)}$$

$$1 < \varepsilon/2\gamma \qquad \text{(A69)}$$

The necessary and sufficient conditions for the arrangement $0<\psi_2<\rho_2<\psi_1<\rho_1$ are as before,

$$\gamma(\vartheta'-\vartheta)^2 < (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon'<\varepsilon$$

In summary, the necessary and sufficient conditions for $0<\psi_2<1<\rho_2<\psi_1<\rho_1$ are

$$\gamma(\vartheta'-\vartheta)^2 < (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon'<\varepsilon$$
$$(\gamma-\varepsilon'+\vartheta')<0$$
$$(\gamma-\varepsilon+\vartheta)>0$$
$$2\gamma<\varepsilon$$

Or in a more compact form,

$$\gamma(\vartheta'-\vartheta)^2 < (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon > \sup(\varepsilon', 2\gamma)$$
$$(\varepsilon-\vartheta) < \gamma < (\varepsilon'-\vartheta')$$

b5] $1<\psi_2<\rho_2<\psi_1<\rho_1$

The necessary and sufficient conditions for 1 to be less than ψ_1, ψ_2 are according to theorem A2,

$$-\gamma G(1) > 0 \quad , \quad 1 < (\psi_1+\psi_2)/2$$

Using (A13), (A3), we can write these conditions as

$$(\gamma-\varepsilon'+\vartheta')>0 \tag{A70}$$

$$1<\varepsilon'/2\gamma \tag{A71}$$

The necessary and sufficient conditions for $\psi_2<\rho_2<\psi_1<\rho_1$ are as before,

$$\gamma(\vartheta'-\vartheta)^2<(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon'<\varepsilon$$

In summary, the necessary and sufficient conditions for the arrangement $1<\psi_2<\rho_2<\psi_1<\rho_1$ are

$$\gamma(\vartheta'-\vartheta)^2<(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon'<\varepsilon$$
$$(\gamma-\varepsilon'+\vartheta')>0$$
$$2\gamma<\varepsilon'$$

Or in a more compact form,

$$\gamma(\vartheta'-\vartheta)^2<(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$2\gamma<\varepsilon'<\varepsilon$$
$$(\gamma-\varepsilon'+\vartheta')>0$$

c1] $0<\rho_2<\psi_2<\psi_1<\rho_1<1$

The necessary and sufficient conditions for $\rho_2<\psi_2<\psi_1<\rho_1$ are according to theorem A7c given by

$$\Delta_G>0$$
$$R_{G\phi}>0$$
$$\gamma\{\phi(\psi_1)+\phi(\psi_2)\}<0$$

Using (A9), (A7), we can write these conditions as

$$\varepsilon'^2-4\gamma\vartheta'>0 \tag{A72}$$

$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta') \tag{A73}$$

$$\varepsilon'(\varepsilon'-\varepsilon) < 2\gamma(\vartheta'-\vartheta) \tag{A74}$$

The necessary and sufficient conditions for zero to be less than ρ_1, ρ_2 are according to theorem A1,

$$\Delta_\phi > 0 \quad , \quad \gamma\phi(0) > 0 \quad , \quad 0 < (\rho_1+\rho_2)/2$$

Using (A10),(A1), we can write these conditions as

$$(\varepsilon^2-4\gamma\vartheta) > 0 \tag{A75}$$

$$\gamma\vartheta > 0 \tag{A76}$$

$$\varepsilon/2\gamma > 0 \tag{A77}$$

Conditions (A76), (A77) are automatically satisfied. Condition (A75) is repetitive, because

$$R_{G\phi} = \gamma^2\,\phi(\Psi_1)\,\phi(\Psi_2) > 0$$

and

$$\gamma\{\phi(\Psi_1)+\phi(\Psi_2)\} < 0$$

imply that

$$\gamma\phi(\Psi_1) < 0$$
$$\gamma\phi(\Psi_2) < 0$$

which according to theorem A5 means that ρ_1, ρ_2 are real and unequal. Therefore, we do not really need to require that $(\varepsilon^2-4\gamma\vartheta) > 0$.

The necessary and sufficient conditions for 1 to be greater than ρ_1, ρ_2 are according to theorem A3,

$$\gamma\phi(1) > 0 \quad , \quad 1 > (\rho_1+\rho_2)/2$$

Using (A11), (A1), we can write these conditions as

$$(\gamma-\varepsilon+\vartheta) > 0 \tag{A78}$$

$$1 > \varepsilon/2\gamma \tag{A79}$$

In summary, the necessary and sufficient conditions for the arrangement $0<\rho_2<\psi_2<\psi_1<\rho_1<1$ are

$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon'(\varepsilon'-\varepsilon)<2\gamma(\vartheta'-\vartheta)$$
$$\gamma>\sup\{\varepsilon/2\,,\,(\varepsilon-\vartheta)\}$$

c2] $0<\rho_2<\psi_2<\psi_1<1<\rho_1$

The necessary and sufficient conditions for the arrangement $0<\rho_2<\psi_2<\psi_1<\rho_1$ are as before

$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon'(\varepsilon'-\varepsilon)<2\gamma(\vartheta'-\vartheta)$$

The necessary and sufficient conditions for 1 to be between ρ_1, ρ_2 are according to theorem A5,

$$\gamma\Phi(1)<0$$

Using (A11), we can write this condition as

$$(\gamma-\varepsilon+\vartheta)<0$$

The necessary and sufficient conditions for 1 to be greater than ψ_1, ψ_2 are according to theorem A4,

$$-\gamma G(1)>0\ , \quad 1>(\psi_1+\psi_2)/2$$

Using (A13), (A3), we can write these conditions as

$$(\gamma-\varepsilon'+\vartheta')>0$$
$$1>\varepsilon'/2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $0<\rho_2<\psi_2<\psi_1<1<\rho_1$ are

$$(\varepsilon'^2 - 4\gamma\vartheta') > 0$$
$$\gamma(\vartheta' - \vartheta)^2 > (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta')$$
$$\varepsilon'(\varepsilon' - \varepsilon) < 2\gamma(\vartheta' - \vartheta)$$
$$\varepsilon' < 2\gamma$$
$$(\varepsilon' - \vartheta') < \gamma < (\varepsilon - \vartheta)$$

c3] $0 < \rho_2 < \Psi_2 < 1 < \Psi_1 < \rho_1$

The necessary and sufficient conditions for the arrangement $0 < \rho_2 < \Psi_2 < \Psi_1 < \rho_1$ are as before

$$\varepsilon'^2 - 4\gamma\vartheta' > 0$$
$$\gamma(\vartheta' - \vartheta)^2 > (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta')$$
$$\varepsilon'(\varepsilon' - \varepsilon) < 2\gamma(\vartheta' - \vartheta)$$

The necessary and sufficient conditions for 1 to be between ρ_1, ρ_2 and Ψ_1, Ψ_2 are according to theorems A5 and A6 given by

$$\gamma\Phi(1) < 0$$
$$-\gamma G(1) < 0$$

Using (A11), (A13), we can write these conditions as

$$(\gamma - \varepsilon + \vartheta) < 0$$
$$(\gamma - \varepsilon' + \vartheta') < 0$$

In summary, the necessary and sufficient conditions for $0 < \rho_2 < \Psi_2 < 1 < \Psi_1 < \rho_1$ are

$$\varepsilon'^2 - 4\gamma\vartheta' > 0$$
$$\gamma(\vartheta' - \vartheta)^2 > (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta')$$
$$\varepsilon'(\varepsilon' - \varepsilon) < 2\gamma(\vartheta' - \vartheta)$$
$$(\gamma - \varepsilon' + \vartheta') < 0$$

c4] $0 < \rho_2 < 1 < \Psi_2 < \Psi_1 < \rho_1$

The necessary and sufficient conditions for the arrangement $0<\rho_2<\psi_2<\psi_1<\rho_1$ are as before

$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon'(\varepsilon'-\varepsilon)<2\gamma(\vartheta'-\vartheta)$$

The necessary and sufficient conditions for 1 to be between ρ_1, ρ_2 are according to theorem A5,

$$\gamma\Phi(1)<0$$

Using (A11), we can write this condition as

$$(\gamma-\varepsilon+\vartheta)<0$$

The necessary and sufficient conditions for 1 to be less than ψ_1 , ψ_2 are according to theorem A2,

$$-\gamma G(1)>0 \quad , \quad 1<(\psi_1+\psi_2)/2$$

Using (A13), (A3), we can write these conditions as

$$(\gamma-\varepsilon'+\vartheta')>0$$
$$1<\varepsilon'/2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $0<\rho_2<1<\psi_2<\psi_1<\rho_1$ are

$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon'(\varepsilon'-\varepsilon)<2\gamma(\vartheta'-\vartheta)$$
$$(\gamma-\varepsilon+\vartheta)<0$$
$$(\gamma-\varepsilon'+\vartheta')>0$$
$$2\gamma<\varepsilon'$$

Or in a more compact form,

$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon'(\varepsilon'-\varepsilon)<2\gamma(\vartheta'-\vartheta)$$
$$(\varepsilon'-\vartheta')<\gamma<(\varepsilon-\vartheta)$$
$$\varepsilon'>2\gamma$$

c5] $1<\rho_2<\psi_2<\psi_1<\rho_1$

The necessary and sufficient conditions for $\rho_2<\psi_2<\psi_1<\rho_1$ are as before,

$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon'(\varepsilon'-\varepsilon)<2\gamma(\vartheta'-\vartheta)$$

The necessary and sufficient conditions for 1 to be less than ρ_1 , ρ_2 are according to theorem A1,

$$\gamma\phi(1)>0\,,\quad 1<(\rho_1+\rho_2)/2$$

Using (A11), (A1), we can write these conditions as

$$(\gamma-\varepsilon+\vartheta)>0$$
$$1<\varepsilon/2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $1<\rho_2<\psi_2<\psi_1<\rho_1$ are

$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon'(\varepsilon'-\varepsilon)<2\gamma(\vartheta'-\vartheta)$$
$$(\varepsilon-\vartheta)<\gamma<\varepsilon/2$$

d1] $0<\psi_2<\rho_2<\rho_1<\psi_1<1$

The necessary and sufficient conditions for $\psi_2<\rho_2<\rho_1<\psi_1$ are according to theorem A7d given by (A23)-(A25). Using (A9), (A8), we can write these conditions as

$$\varepsilon^2-4\gamma\vartheta>0 \qquad \text{(A80)}$$

$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta') \qquad \text{(A81)}$$

$$\varepsilon(\varepsilon'-\varepsilon)>2\gamma(\vartheta'-\vartheta) \qquad \text{(A82)}$$

The necessary and sufficient conditions for zero to be less than ψ_1, ψ_2 are according to theorem A2,

$$\Delta_{G} > 0 \quad , \quad -\gamma G(0) > 0 \quad , \quad 0 < (\psi_1 + \psi_2)/2$$

Using (A12), (A3), we can write these conditions as

$$\varepsilon'^2 - 4\gamma\vartheta' > 0 \qquad \text{(A83)}$$

$$\gamma\vartheta' > 0 \qquad \text{(A84)}$$

$$\varepsilon'/2\gamma > 0 \qquad \text{(A85)}$$

Since γ, ϑ' and ε' are positive by definition, (A84)-(A85) are automatically satisfied. Condition (A83) is repetitious, because

$$R_{G\phi} = \gamma^2 G(p_1) G(p_2) > 0$$
$$-\gamma\{G(p_1) + G(p_2)\} < 0$$

imply that

$$-\gamma G(p_1) < 0$$
$$-\gamma G(p_2) < 0$$

which according to theorem A6 means that ψ_1, ψ_2 are real and unequal. Therefore, we do not need to require that $\varepsilon'^2 - 4\gamma\vartheta' > 0$, because conditions (A81)-(A82) guarantee this.

The necessary and sufficient conditions for 1 to be greater than ψ_1, ψ_2 are according to theorem A4,

$$-\gamma G(1) > 0 \quad , \quad 1 > (\psi_1 + \psi_2)/2$$

Using (A13), (A3), we can write these conditions as

$$(\gamma - \varepsilon' + \vartheta') > 0$$
$$1 > \varepsilon'/2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $0<\Psi_2<\rho_2<\rho_1<\Psi_1<1$ are

$$\varepsilon^2-4\gamma\vartheta>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon(\varepsilon'-\varepsilon)>2\gamma(\vartheta'-\vartheta)$$
$$\gamma>\sup\{\varepsilon'/2,(\varepsilon'-\vartheta')\}$$

d2] $0<\Psi_2<\rho_2<\rho_1<1<\Psi_1$

The necessary and sufficient conditions for 1 to be between Ψ_1, Ψ_2 are according to theorem A6,

$$-\gamma G(1)<0$$

Using (A13),

$$(\gamma-\varepsilon'+\vartheta')<0$$

The necessary and sufficient conditions for 1 to be greater than ρ_1 , ρ_2 are according to theorem A3

$$\gamma\phi(1)>0 \quad , \quad 1>(\rho_1+\rho_2)/2$$

Using (A11), (A1),

$$(\gamma-\varepsilon+\vartheta)>0$$
$$1>\varepsilon/2\gamma$$

The necessary and sufficient conditions for $0<\Psi_2<\rho_2<\rho_1<\Psi_1$ are (A80)-(A82).

In summary, the necessary and sufficient conditions for the arrangement $0<\Psi_2<\rho_2<\rho_1<1<\Psi_1$ are

$$\varepsilon^2-4\gamma\vartheta>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon(\varepsilon'-\varepsilon)>2\gamma(\vartheta'-\vartheta)$$
$$\sup\{\tfrac{\varepsilon}{2},(\varepsilon-\vartheta)\}<\gamma<(\varepsilon'-\vartheta')$$

d3] $0<\psi_2<\rho_2<1<\rho_1<\psi_1$

The necessary and sufficient conditions for $0<\psi_2<\rho_2<\rho_1<\psi_1$ are (A80)-(A82).

The necessary and sufficient conditions for 1 to be between ρ_1, ρ_2 are according to theorem A5,

$$\gamma\Phi(1)<0$$

Using (A11),

$$(\gamma-\varepsilon+\vartheta)<0$$

In summary, the necessary and sufficient conditions for the arrangement $0<\psi_2<\rho_2<1<\rho_1<\psi_1$ are,

$$\varepsilon^2-4\gamma\vartheta>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon(\varepsilon'-\varepsilon)>2\gamma(\vartheta'-\vartheta)$$
$$(\gamma-\varepsilon+\vartheta)<0$$

d4] $0<\psi_2<1<\rho_2<\rho_1<\psi_1$

The necessary and sufficient conditions for $0<\psi_2<\rho_2<\rho_1<\psi_1$ are (A80)-(A82).

The necessary and sufficient condotions for 1 to lie between ψ_1, ψ_2 are according to theorem A6,

$$-\gamma G(1)<0$$

Using (A13),

$$(\gamma-\varepsilon'+\vartheta')<0$$

The necessary and sufficient conditions for 1 to be less than ρ_1, ρ_2 are according to theorem A1,

$$\gamma\Phi(1)>0, \quad 1<(\rho_1+\rho_2)/2$$

Using (A11), (A1),

$$(\gamma-\varepsilon+\vartheta)>0$$
$$1<\varepsilon/2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $0<\psi_2<1<\rho_2<\rho_1<\psi_1$ are

$$\varepsilon^2-4\gamma\vartheta>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon(\varepsilon'-\varepsilon)>2\gamma(\vartheta'-\vartheta)$$
$$(\varepsilon-\vartheta)<\gamma<\inf\{\varepsilon/2,(\varepsilon'-\vartheta')\}$$

d5] $1<\psi_2<\rho_2<\rho_1<\psi_1$

The necessary and sufficient conditions for $\psi_2<\rho_2<\rho_1<\psi_1$ are (A80)-(A82).

The necessary and sufficient conditions for 1 to be less than ψ_1,ψ_2 are according to theorem A2,

$$-\gamma G(1)>0, \quad 0<(\psi_1+\psi_2)/2$$

Using (A13), (A3),

$$(\gamma-\varepsilon'+\vartheta')>0$$
$$0<\varepsilon'/2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $1<\psi_2<\rho_2<\rho_1<\psi_1$ are,

$$\varepsilon^2-4\gamma\vartheta>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon(\varepsilon'-\varepsilon)>2\gamma(\vartheta'-\vartheta)$$
$$(\varepsilon'-\vartheta')<\gamma<\frac{\varepsilon'}{2}$$

e1] $0<\rho_2<\rho_1<\psi_2<\psi_1<1$

The necessary and sufficientconditions for $0<\rho_2<\rho_1<\psi_2<\psi_1$ are according to theorem A7e,

$$\Delta_\phi > 0, \; \Delta_G > 0, \; R_{G\phi} > 0$$
$$\gamma\{\Phi(\Psi_1) + \Phi(\Psi_2)\} > 0$$
$$-\gamma\{G(\rho_1) + G(\rho_2)\} > 0$$
$$\rho_1 + \rho_2 < \Psi_1 + \Psi_2$$

Using (A9),(A7), (A8), (A1), (A3), we can write these conditions as

$$\varepsilon^2 - 4\gamma\vartheta > 0 \tag{A86}$$

$$\varepsilon'^2 - 4\gamma\vartheta' > 0 \tag{A87}$$

$$\gamma(\vartheta' - \vartheta)^2 > (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta') \tag{A88}$$

$$\varepsilon'(\varepsilon' - \varepsilon) > 2\gamma(\vartheta' - \vartheta) \tag{A89}$$

$$\varepsilon(\varepsilon' - \varepsilon) < 2\gamma(\vartheta' - \vartheta) \tag{A90}$$

$$\varepsilon < \varepsilon' \tag{A91}$$

The necessary and sufficient conditions for 1 to be greater than Ψ_1, Ψ_2 are according to theorem A4,

$$-\gamma G(1) > 0 \quad , \quad 1 > (\Psi_1 + \Psi_2)/2$$

Using (A13), (A3),

$$(\gamma - \varepsilon' + \vartheta') > 0$$
$$1 > \varepsilon'/2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $0 < \rho_2 < \rho_1 < \Psi_2 < \Psi_1 < 1$ are

$$\varepsilon^2 - 4\gamma\vartheta > 0$$
$$\varepsilon'^2 - 4\gamma\vartheta' > 0$$
$$\gamma(\vartheta' - \vartheta)^2 > (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta')$$
$$\varepsilon(\varepsilon' - \varepsilon) < 2\gamma(\vartheta' - \vartheta) < \varepsilon'(\varepsilon' - \varepsilon)$$
$$\varepsilon < \varepsilon' < 2\gamma$$
$$(\gamma - \varepsilon' + \vartheta') > 0$$

e2] $0 < \rho_2 < \rho_1 < \Psi_2 < 1 < \Psi_1$

The necessary and sufficient conditions for $0 < \rho_2 < \rho_1 < \Psi_2 < \Psi_1$ are (A86)-(A91).

The necessary and sufficient conditions for 1 to lie between Ψ_1, Ψ_2 are according to theorem A6,

$$-\gamma G(1) < 0$$

Using (A13),

$$(\gamma - \varepsilon' + \vartheta') < 0$$

In summary, the necessary and sufficient conditions for the arrangement $0 < \rho_2 < \rho_1 < \Psi_2 < 1 < \Psi_1$ are,

$$\varepsilon^2 - 4\gamma\vartheta > 0$$
$$\varepsilon'^2 - 4\gamma\vartheta' > 0$$
$$\gamma(\vartheta' - \vartheta)^2 > (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta')$$
$$\varepsilon(\varepsilon' - \varepsilon) < 2\gamma(\vartheta' - \vartheta) < \varepsilon'(\varepsilon' - \varepsilon)$$
$$\varepsilon < \varepsilon'$$
$$(\gamma - \varepsilon' + \vartheta') < 0$$

e3] $0 < \rho_2 < \rho_1 < 1 < \Psi_2 < \Psi_1$

The necessary and sufficient conditions for $0 < \rho_2 < \rho_1 < \Psi_2 < \Psi_1$ are (A86)-(A91).

The necessary and sufficient conditions for 1 to be less than Ψ_1 , Ψ_2 are according to theorem A2

$$-\gamma G(1) > 0 , \quad 1 < (\psi_1+\psi_2)/2$$

Using (A13), (A3),

$$(\gamma-\varepsilon'+\vartheta') > 0$$
$$1 < \varepsilon'/2\gamma$$

The necessary and sufficient conditions for 1 to be greater than ρ_1, ρ_2 are according to theorem A3,

$$\gamma\Phi(1) > 0, \quad 1 > (\rho_1+\rho_2)/2$$

Using (A11), (A1),

$$(\gamma-\varepsilon+\vartheta) > 0$$
$$1 > \varepsilon/2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $0<\rho_2<\rho_1<1<\psi_2<\psi_1$ are,

$$\varepsilon^2-4\gamma\vartheta > 0$$
$$\varepsilon'^2-4\gamma\vartheta' > 0$$
$$\gamma(\vartheta'-\vartheta)^2 > (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon(\varepsilon'-\varepsilon) < 2\gamma(\vartheta'-\vartheta) < \varepsilon'(\varepsilon'-\varepsilon)$$
$$\sup\{(\varepsilon'-\vartheta'), (\varepsilon-\vartheta), \tfrac{\varepsilon}{2}\} < \gamma < \frac{\varepsilon'}{2}$$

e4] $0<\rho_2<1<\rho_1<\psi_2<\psi_1$

The necessary and sufficient conditions for $0<\rho_2<\rho_1<\psi_2<\psi_1$ are (A86)-(A91).

The necessary and sufficient conditions for 1 to lie between ρ_1, ρ_2 are according to theorem A5,

$$\gamma\Phi(1) < 0$$

Using (A11),

$$(\gamma-\varepsilon+\vartheta) < 0$$

In summary, the necessary and sufficient conditions for the arrangement $0 < \rho_2 < 1 < \rho_1 < \Psi_2 < \Psi_1$ are

$$\varepsilon^2 - 4\gamma\vartheta > 0$$
$$\varepsilon'^2 - 4\gamma\vartheta' > 0$$
$$\gamma(\vartheta' - \vartheta)^2 > (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta')$$
$$\varepsilon(\varepsilon' - \varepsilon) < 2\gamma(\vartheta' - \vartheta) < \varepsilon'(\varepsilon' - \varepsilon)$$
$$\varepsilon < \varepsilon'$$
$$(\gamma - \varepsilon + \vartheta) < 0$$

e5] $1 < \rho_2 < \rho_1 < \Psi_2 < \Psi_1$

The necessary and sufficient conditions for $\rho_2 < \rho_1 < \Psi_2 < \Psi_1$ are (A86)-(A91).

The necessary and sufficient conditions for 1 to be less than ρ_1, ρ_2 are according to theorem A1,

$$\gamma\Phi(1) > 0 \quad , \quad 1 < (\rho_1 + \rho_2)/2$$

Using (A11), (A1),

$$(\gamma - \varepsilon + \vartheta) > 0$$
$$1 < \varepsilon/2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $1 < \rho_2 < \rho_1 < \Psi_2 < \Psi_1$ are,

$$\varepsilon^2 - 4\gamma\vartheta > 0$$
$$\varepsilon'^2 - 4\gamma\vartheta' > 0$$
$$\gamma(\vartheta' - \vartheta)^2 > (\varepsilon - \varepsilon')(\varepsilon'\vartheta - \varepsilon\vartheta')$$
$$\varepsilon(\varepsilon' - \varepsilon) < 2\gamma(\vartheta' - \vartheta) < \varepsilon'(\varepsilon' - \varepsilon)$$
$$2\gamma < \varepsilon < \varepsilon'$$
$$(\gamma - \varepsilon + \vartheta) > 0$$

f1] $0<\psi_2<\psi_1<\rho_2<\rho_1<1$

The necessary and sufficient conditions for $0<\psi_2<\psi_1<\rho_2<\rho_1$ are according to theorem A7f,

$$\Delta_\phi>0\ ,\ \Delta_G>0\ ,\ R_{G\phi}>0$$

$$\gamma\{\phi(\psi_1)+\phi(\psi_2)\}>0$$

$$-\gamma\{G(\rho_1)+G(\rho_2)\}>0$$

$$\psi_1+\psi_2<\rho_1+\rho_2$$

Using (A9), (A7), (A8), (A1), (A3), we can write these conditions as

$$\varepsilon^2-4\gamma\vartheta>0 \qquad \text{(A92)}$$

$$\varepsilon'^2-4\gamma\vartheta'>0 \qquad \text{(A93)}$$

$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta') \qquad \text{(A94)}$$

$$\varepsilon'(\varepsilon'-\varepsilon)>2\gamma(\vartheta'-\vartheta) \qquad \text{(A95)}$$

$$\varepsilon(\varepsilon'-\varepsilon)<2\gamma(\vartheta'-\vartheta) \qquad \text{(A96)}$$

$$\varepsilon>\varepsilon' \qquad \text{(A97)}$$

The necessary and sufficient conditions for 1 to be greater than ρ_1 , ρ_2 are according to theorem A3,

$$\gamma\phi(1)>0 \quad , \quad 1>(\rho_1+\rho_2)/2$$

Using (A11), (A1),

$$(\gamma-\varepsilon+\vartheta)>0$$

$$1>\varepsilon/2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $0<\psi_2<\psi_1<\rho_2<\rho_1<1$ are,

$$\varepsilon^2-4\gamma\vartheta>0$$
$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon(\varepsilon'-\varepsilon)<2\gamma(\vartheta'-\vartheta)<\varepsilon'(\varepsilon'-\varepsilon)$$
$$2\gamma>\varepsilon>\varepsilon'$$
$$(\gamma-\varepsilon+\vartheta)>0$$

f2] $0<\psi_2<\psi_1<\rho_2<1<\rho_1$

The necessary and sufficient conditions for $0<\psi_2<\psi_1<\rho_2<\rho_1$ are (A92)-(A97).

The necessary and sufficient conditions for 1 to be between ρ_1, ρ_2 are according to theorem A5,

$$\gamma\Phi(1)<0$$

Using (A11),

$$(\gamma-\varepsilon+\vartheta)<0$$

In summary, the necessary and sufficient conditions for the arrangement $0<\psi_2<\psi_1<\rho_2<1<\rho_1$ are,

$$\varepsilon^2-4\gamma\vartheta>0$$
$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon(\varepsilon'-\varepsilon)<2\gamma(\vartheta'-\vartheta)<\varepsilon'(\varepsilon'-\varepsilon)$$
$$\varepsilon>\varepsilon'$$
$$(\gamma-\varepsilon+\vartheta)<0$$

f3] $0<\psi_2<\psi_1<1<\rho_2<\rho_1$

The necessary and sufficient conditions for $0<\psi_2<\psi_1<\rho_2<\rho_1$

are (A92)-(A97).

The necessary and sufficient conditions for 1 to be less than ρ_1, ρ_2 are according to theorem A1,

$$\gamma\Phi(1) > 0 \quad , \quad 1 < (\rho_1+\rho_2)/2$$

Using (A11), (A1), we can write these conditions as

$$(\gamma-\varepsilon+\vartheta) > 0$$
$$1 < \varepsilon/2\gamma$$

The necessary and sufficient conditions for 1 to be greater than ψ_1, ψ_2 are according to theorem A4,

$$-\gamma G(1) > 0 \quad , \quad 1 > (\psi_1+\psi_2)/2$$

Using (A13), (A3),

$$(\gamma-\varepsilon'+\vartheta') > 0$$
$$1 > \varepsilon'/2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $0<\psi_2<\psi_1<1<\rho_2<\rho_1$ are

$$\varepsilon^2-4\gamma\vartheta > 0$$
$$\varepsilon'^2-4\gamma\vartheta' > 0$$
$$\gamma(\vartheta'-\vartheta)^2 > (\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon(\varepsilon'-\varepsilon) < 2\gamma(\vartheta'-\vartheta) < \varepsilon'(\varepsilon'-\varepsilon)$$
$$\sup\left\{(\varepsilon-\vartheta),(\varepsilon'-\vartheta'),\frac{\varepsilon'}{2}\right\} < \gamma < \frac{\varepsilon}{2} .$$

f4] $0<\psi_2<1<\psi_1<\rho_2<\rho_1$

The necessary and sufficient conditions for $0<\psi_2<\psi_1<\rho_2<\rho_1$ are (A92)-(A97).

The necessary and sufficient conditions for 1 to lie between ψ_1, ψ_2 are according to theorem A6,

$$-\gamma G(1) < 0$$

Using (A13),

$$(\gamma-\varepsilon'+\vartheta')<0$$

In summary, the necessary and sufficient conditions for the arrangement $0<\psi_2<1<\psi_1<\rho_2<\rho_1$ are

$$\varepsilon^2-4\gamma\vartheta>0$$
$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon(\varepsilon'-\varepsilon)<2\gamma(\vartheta'-\vartheta)<\varepsilon'(\varepsilon'-\varepsilon)$$
$$\varepsilon'<\varepsilon$$
$$(\gamma-\varepsilon'+\vartheta')<0$$

f5] $1<\psi_2<\psi_1<\rho_2<\rho_1$

The necessary and sufficient conditions for $\psi_2<\psi_1<\rho_2<\rho_1$ are (A92)-(A97).

The necessary and sufficient conditions for 1 to be less than ψ_1, ψ_2 are according to theorem A2,

$$-\gamma G(1)>0 \quad , \quad 1<(\psi_1+\psi_2)/2$$

Using (A13), (A3),

$$(\gamma-\varepsilon'+\vartheta')>0$$
$$1<\varepsilon'/2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $1<\psi_2<\psi_1<\rho_2<\rho_1$ are,

$$\varepsilon^2-4\gamma\vartheta>0$$
$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$\gamma(\vartheta'-\vartheta)^2>(\varepsilon-\varepsilon')(\varepsilon'\vartheta-\varepsilon\vartheta')$$
$$\varepsilon(\varepsilon'-\varepsilon)<2\gamma(\vartheta'-\vartheta)<\varepsilon'(\varepsilon'-\varepsilon)$$
$$2\gamma<\varepsilon'<\varepsilon$$
$$(\gamma-\varepsilon'+\vartheta')>0$$

CASE B

a1] $0<\rho<\Psi_2<\Psi_1<1$

The necessary and sufficient condition for $\Phi(\xi)=0$ to have a double root, $\rho=\varepsilon/2\gamma$, is

$$\varepsilon^2=4\gamma\vartheta \tag{A98}$$

The necessary and sufficient conditions for $0<\rho<\Psi_2<\Psi_1$ are according to theorem A2,

$$\Delta_G>0\ ,\ -\gamma G(\varepsilon/2\gamma)>0\ ,\ \frac{\varepsilon}{2\gamma}<(\Psi_1+\Psi_2)/2$$

Using (A14), (A3), we can write these conditions as

$$\varepsilon'^2-4\gamma\vartheta'>0 \tag{A99}$$

$$2\gamma\vartheta'>\varepsilon\left(\varepsilon'-\frac{\varepsilon}{2}\right) \tag{A100}$$

$$\varepsilon<\varepsilon' \tag{A101}$$

The necessary and sufficient conditions for 1 to be greater than Ψ_1 , Ψ_2 are according to thoerem A4,

$$-\gamma G(1)>0\ ,\ 1>(\Psi_1+\Psi_2)/2$$

Using (A13), (A3),

$$(\gamma-\varepsilon'+\vartheta')>0$$
$$1>\varepsilon'/2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $o<\rho<\Psi_2<\Psi_1<1$ are

$$\varepsilon^2=4\gamma\vartheta$$
$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$2\gamma\vartheta'>\varepsilon(\varepsilon'-\frac{\varepsilon}{2})$$
$$\varepsilon<\varepsilon'<2\gamma$$
$$(\gamma-\varepsilon'+\vartheta')>0$$

a2] $o<\rho<\Psi_2<1<\Psi_1$

The necessary and sufficient conditions for $o<\rho<\Psi_2<\Psi_1$ are (A98)-(A101).

The necessary and sufficient condition for 1 to lie between Ψ_1, Ψ_2 is according to theorem A6,

$$-\gamma G(1)<0$$

Using (A13),

$$(\gamma-\varepsilon'+\vartheta')<0$$

In summary, the necessary and sufficient conditions for the arrangement $o<\rho<\Psi_2<1<\Psi_1$ are

$$\varepsilon^2=4\gamma\vartheta$$
$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$2\gamma\vartheta'>\varepsilon(\varepsilon'-\frac{\varepsilon}{2})$$
$$\varepsilon<\varepsilon'$$
$$(\gamma-\varepsilon'+\vartheta')<0$$

a3] $o<\rho<1<\Psi_2<\Psi_1$

The necessary and sufficient conditions for $o<\rho<\Psi_2<\Psi_1$ are (A98)-(A101).

The necessary and sufficient conditions for 1 to be less than Ψ_1, Ψ_2 and greater than ρ are according to theorem A2,

$$-\gamma G(1) > 0 \quad , \quad 1 < (\Psi_1 + \Psi_2)/2 \quad , \quad \varepsilon < 2\gamma$$

Using (A13), (A3),

$$(\gamma - \varepsilon' + \vartheta') > 0$$
$$1 < \varepsilon'/2\gamma$$
$$\varepsilon < 2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $0 < \rho < 1 < \Psi_2 < \Psi_1$ are,

$$\varepsilon^2 = 4\gamma\vartheta$$
$$\varepsilon'^2 - 4\gamma\vartheta' > 0$$
$$2\gamma\vartheta' > \varepsilon\left(\varepsilon' - \frac{\varepsilon}{2}\right)$$
$$\sup\left\{(\varepsilon' - \vartheta'), \frac{\varepsilon}{2}\right\} < \gamma < \frac{\varepsilon'}{2}$$

a4] $1 < \rho < \Psi_2 < \Psi_1$

The necessary and sufficient conditions for $\rho < \Psi_2 < \Psi_1$ are (A98)-(A101).

The necessary and sufficient condition for 1 to be less than ρ is

$$\varepsilon > 2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $1 < \rho < \Psi_2 < \Psi_1$ are,

$$\varepsilon^2 = 4\gamma\vartheta,$$
$$\varepsilon'^2 - 4\gamma\vartheta' > 0$$
$$2\gamma\vartheta' > \varepsilon\left(\varepsilon' - \frac{\varepsilon}{2}\right)$$
$$2\gamma < \varepsilon < \varepsilon'$$

b1] $0 < \Psi_2 < \Psi_1 < \rho < 1$

The necessary and sufficient conditions for $0 < \Psi_2 < \Psi_1 < \rho$, where ρ is a double root of the equation $\Phi(\xi)=0$,

are according to theorem A4,

$$\varepsilon^2=4\gamma\vartheta,\quad -\gamma G(\varepsilon/2\gamma)>0,\quad \frac{\varepsilon}{2\gamma}>(\psi_1+\psi_2)/2,\quad \Delta_G>0$$

Using (A14), (A3), we can write these conditions as

$$\varepsilon^2=4\gamma\vartheta \tag{A102}$$

$$\varepsilon'^2-4\gamma\vartheta'>0 \tag{A103}$$

$$2\gamma\vartheta'>\varepsilon\left(\varepsilon'-\frac{\varepsilon}{2}\right) \tag{A104}$$

$$\varepsilon>\varepsilon' \tag{A105}$$

The necessary and sufficient condition for 1 to be greater than ρ is,

$$\varepsilon<2\gamma$$

In summary, the necesssary and sufficient conditions for the arrangement $0<\psi_2<\psi_1<\rho<1$ are

$$\varepsilon^2=4\gamma\vartheta$$
$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$2\gamma\vartheta'>\varepsilon\left(\varepsilon'-\frac{\varepsilon}{2}\right)$$
$$\varepsilon'<\varepsilon<2\gamma$$

b2] $0<\psi_2<\psi_1<1<\rho$

The necessary and sufficient conditions for $0<\psi_2<\psi_1<\rho$ are (A102)-(A105).

The necessary and sufficient conditions for 1 to be greater than ψ_1,ψ_2 and less than ρ, are according to theorem A4,

$$-\gamma G(1)>0,\quad 1>(\psi_1+\psi_2)/2,\quad \varepsilon>2\gamma$$

Using (A13), (A3),

$$(\gamma-\varepsilon'+\vartheta')>0$$
$$1>\varepsilon'/2\gamma$$
$$\varepsilon>2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $0<\Psi_2<\Psi_1<1<\rho$ are,

$$\varepsilon^2=4\gamma\vartheta$$
$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$2\gamma\vartheta'>\varepsilon\left(\varepsilon'-\frac{\varepsilon}{2}\right)$$
$$\sup\{(\varepsilon'-\vartheta'),\varepsilon'/2\}<\gamma<\frac{\varepsilon}{2}$$

b3] $0<\Psi_2<1<\Psi_1<\rho$

The necessary and sufficient conditions for $0<\Psi_2<\Psi_1<\rho$ are (A102)-(A105).

The necessary and sufficient conditions for 1 to lie between Ψ_1 , Ψ_2 are according to theorem A6,

$$-\gamma G(1)<0$$

Using (A13),

$$(\gamma-\varepsilon'+\vartheta')<0$$

In summary, the necessary and sufficient conditions for the arrangement $0<\Psi_2<1<\Psi_1<\rho$ are,

$$\varepsilon^2=4\gamma\vartheta$$
$$\varepsilon'^2-4\gamma\vartheta'>0$$
$$2\gamma\vartheta'>\varepsilon\left(\varepsilon'-\frac{\varepsilon}{2}\right)$$
$$\varepsilon'<\varepsilon$$
$$(\gamma-\varepsilon'+\vartheta')<0$$

b4] $1 < \Psi_2 < \Psi_1 < \rho$

The necessary and sufficient conditions for $\Psi_2 < \Psi_1 < \rho$ are (A102)-(A105).

The necessary and sufficient conditions for 1 to be less than Ψ_1 , Ψ_2 , are according to theorem A2,

$$-\gamma G(1) > 0 \quad , \quad 1 < (\Psi_1 + \Psi_2)/2$$

Using (A13),(A3),

$$(\gamma - \varepsilon' + \vartheta') > 0$$

$$1 < \varepsilon'/2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $1 < \Psi_2 < \Psi_1 < \rho$ are,

$$\varepsilon^2 = 4\gamma\vartheta$$
$$\varepsilon'^2 - 4\gamma\vartheta' > 0$$
$$2\gamma\vartheta' > \varepsilon(\varepsilon' - \frac{\varepsilon}{2})$$
$$2\gamma < \varepsilon' < \varepsilon$$
$$(\gamma - \varepsilon' + \vartheta') > 0$$

c1] $0 < \Psi_2 < \rho < \Psi_1 < 1$

The necessary and sufficient conditions for $0 < \Psi_2 < \rho < \Psi_1$, where ρ is a double root of $\Phi(\xi) = 0$, are according to theorem A6,

$$\varepsilon^2 = 4\gamma\vartheta \quad , \quad -\gamma G(\varepsilon/2\gamma) < 0$$

Using (A14),

$$\varepsilon^2 = 4\gamma\vartheta \tag{A106}$$

$$2\gamma\vartheta' < \varepsilon(\varepsilon' - \frac{\varepsilon}{2}) \tag{A107}$$

The necessary and sufficient conditions for 1 to be greater than ψ_1 , ψ_2 are according to theorem A4,

$$\Delta_G > 0 \tag{A108}$$

$$-\gamma G(1) > 0 \tag{A109}$$

$$1 > \varepsilon'/2\gamma \tag{A110}$$

Condition (A108) is repetitious, because according to theorem A6, the condition $-\gamma G(\varepsilon/2\gamma) < 0$ guarantees that ψ_1 , ψ_2 are real and unequal. Thus, we can disregard (A108).

Using (A13), we can write (A109)-(A110) as

$$(\gamma - \varepsilon' + \vartheta') > 0$$
$$\varepsilon' < 2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $0 < \psi_2 < \rho < \psi_1 < 1$ are,

$\varepsilon^2 = 4\gamma\vartheta$

$2\gamma\vartheta' < \varepsilon(\varepsilon' - \frac{\varepsilon}{2})$

$\gamma > \sup\{\varepsilon'/2, (\varepsilon' - \vartheta')\}$

c2] $0 < \psi_2 < \rho < 1 < \psi_1$

The necessary and sufficient conditions for $0 < \psi_2 < \rho < \psi_1$ are (A106)-(A107).

The necessary and sufficient conditions for 1 to be between ψ_1 , ψ_2 and greater than ρ are according to theorem A6,

$$-\gamma G(1) < 0$$
$$\varepsilon < 2\gamma$$

Using (A13),

$$(\gamma - \varepsilon' + \vartheta') < 0$$
$$\varepsilon < 2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $0 < \Psi_2 < \rho < 1 < \Psi_1$ are,

$$\varepsilon^2 = 4\gamma\vartheta$$
$$2\gamma\vartheta' < \varepsilon(\varepsilon' - \tfrac{\varepsilon}{2})$$
$$\tfrac{\varepsilon}{2} < \gamma < (\varepsilon' - \vartheta')$$

c3] $0 < \Psi_2 < 1 < \rho < \Psi_1$

The necessary and sufficient conditions for $0 < \Psi_2 < \rho < \Psi_1$ are (A106)-(A107).

The necessary and sufficient conditions for 1 to be between Ψ_1, Ψ_2 and less than ρ are according to theorem A6,

$$-\gamma G(1) < 0$$
$$\varepsilon > 2\gamma$$

Using (A13),

$$(\gamma - \varepsilon' + \vartheta') < 0$$
$$\varepsilon > 2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $0 < \Psi_2 < 1 < \rho < \Psi_1$ are,

$$\varepsilon^2 = 4\gamma\vartheta$$
$$2\gamma\vartheta' < \varepsilon(\varepsilon' - \tfrac{\varepsilon}{2})$$
$$\gamma < \inf\{\varepsilon/2, (\varepsilon' - \vartheta')\}$$

c4] $1<\psi_2<\rho<\psi_1$

The necessary and sufficient conditions for $\psi_2<\rho<\psi_1$ are (A106)-(A107).

The necessary and sufficient conditions for 1 to be less than ψ_1, ψ_2 are according to theorem A2,

$$-\gamma G(1)>0 \quad , \quad 1<(\psi_1+\psi_2)/2$$

Using (A13), (A3),

$$(\gamma-\varepsilon'+\vartheta')>0$$
$$1<\varepsilon'/2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $1<\psi_2<\rho<\psi_1$ are,

$$\varepsilon^2=4\gamma\vartheta$$
$$2\gamma\vartheta'<\varepsilon\left(\varepsilon'-\frac{\varepsilon}{2}\right)$$
$$(\varepsilon'-\vartheta')<\gamma<\varepsilon/2$$

d1] $0<\psi<\rho_2<\rho_1<1$

The necessary and sufficient conditions for $0<\psi<\rho_2<\rho_1$, where ψ is a double root of $G(\omega)=0$, are according to theorem A1,

$$\varepsilon'^2=4\gamma\vartheta'$$
$$\varepsilon^2-4\gamma\vartheta>0$$
$$\gamma\Phi(\varepsilon'/2\gamma)>0$$
$$\varepsilon'/2\gamma<(\rho_1+\rho_2)/2$$

Using (A15), (A1), we can write these conditions as

$$\varepsilon'^2=4\gamma\vartheta' \qquad \text{(A111)}$$

$$\varepsilon^2 - 4\gamma\vartheta > 0 \qquad \text{(A112)}$$

$$2\gamma\vartheta > \varepsilon'(\varepsilon - \frac{\varepsilon'}{2}) \qquad \text{(A113)}$$

$$\varepsilon' < \varepsilon \qquad \text{(A114)}$$

The necessary and sufficient conditions for 1 to be greater than ρ_1, ρ_2, are according to theorem A3,

$$\gamma\Phi(1) > 0\ , \quad 1 > (\rho_1 + \rho_2)/2$$

Using (A11), (A1),

$$(\gamma - \varepsilon + \vartheta) > 0$$
$$1 > \varepsilon/2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $0 < \Psi < \rho_2 < \rho_1 < 1$ are,

$$\varepsilon'^2 = 4\gamma\vartheta'$$
$$\varepsilon^2 - 4\gamma\vartheta > 0$$
$$2\gamma\vartheta > \varepsilon'(\varepsilon - \frac{\varepsilon'}{2})$$
$$\varepsilon' < \varepsilon < 2\gamma$$
$$(\gamma - \varepsilon + \vartheta) > 0$$

d2] $0 < \Psi < \rho_2 < 1 < \rho_1$

The necessary and sufficient conditions for $0 < \Psi < \rho_2 < \rho_1$ are (A111)-(A114).

The necessary and sufficient conditions for 1 to lie between ρ_1, ρ_2 are according to theorem A5,

$$\gamma\Phi(1) < 0$$

Using (A11),

$$(\gamma - \varepsilon + \vartheta) < 0$$

In summary, the necessary and sufficient conditions for the arrangement $0<\Psi<\rho_2<1<\rho_1$ are,

$$\varepsilon'^2 = 4\gamma\vartheta'$$
$$\varepsilon^2-4\gamma\vartheta>0$$
$$2\gamma\vartheta>\varepsilon'(\varepsilon-\frac{\varepsilon'}{2})$$
$$\varepsilon'<\varepsilon$$
$$(\gamma-\varepsilon+\vartheta)<0$$

d3] $0<\Psi<1<\rho_2<\rho_1$

The necessary and sufficient conditions for $0<\Psi<\rho_2<\rho_1$ are (A11)-(A14).

The necessary and sufficient conditions for 1 to be less than ρ_1, ρ_2 and greater than Ψ are according to theorem A1,

$$\gamma\phi(1)>0 \quad , \quad 1<(\rho_1+\rho_2)/2 \quad , \quad \varepsilon'<2\gamma$$

Using (A11), (A1),

$$(\gamma-\varepsilon+\vartheta)>0$$
$$1<\varepsilon/2\gamma$$
$$\varepsilon'<2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $0<\Psi<1<\rho_2<\rho_1$ are,

$$\varepsilon'^2=4\gamma\vartheta'$$
$$\varepsilon^2-4\gamma\vartheta>0$$
$$2\gamma\vartheta>\varepsilon'(\varepsilon-\frac{\varepsilon'}{2})$$
$$\sup\{\varepsilon'/2,(\varepsilon-\vartheta)\}<\gamma<\varepsilon/2$$

d4] $1<\Psi<\rho_2<\rho_1$

The necessary and sufficient conditions for $\Psi<\rho_2<\rho_1$ are (A11)-(A14).

The necessary and sufficient condition for 1 to be less than Ψ is,

$$\varepsilon' > 2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $1 < \Psi < \rho_2 < \rho_1$ are,

$$\varepsilon'^2 = 4\gamma\vartheta'$$
$$\varepsilon^2 - 4\gamma\vartheta > 0$$
$$2\gamma\vartheta > \varepsilon'(\varepsilon - \frac{\varepsilon'}{2})$$
$$2\gamma < \varepsilon' < \varepsilon$$

el] $0 < \rho_2 < \rho_1 < \Psi < 1$

The necessary and sufficient conditions for $0 < \rho_2 < \rho_1 < \Psi$ are according to theorem A3,

$$\varepsilon'^2 = 4\gamma\vartheta'$$
$$\varepsilon^2 - 4\gamma\vartheta > 0$$
$$\gamma\Phi(\varepsilon'/2\gamma) > 0$$
$$\varepsilon'/2\gamma > (\rho_1 + \rho_2)/2$$

Using (A15), (A1),

$$\varepsilon'^2 = 4\gamma\vartheta' \qquad \text{(A115)}$$

$$\varepsilon^2 - 4\gamma\vartheta > 0 \qquad \text{(A116)}$$

$$2\gamma\vartheta > \varepsilon'(\varepsilon - \frac{\varepsilon'}{2}) \qquad \text{(A117)}$$

$$\varepsilon' > \varepsilon \qquad \text{(A118)}$$

The necessary and sufficient condition for 1 to be greater than Ψ is $\varepsilon' < 2\gamma$

In summary, the necessary and sufficient conditions for the arrangement $0 < \rho_2 < \rho_1 < \Psi < 1$ are,

$$\varepsilon'^2 = 4\gamma\vartheta'$$
$$\varepsilon^2 - 4\gamma\vartheta > 0$$
$$2\gamma\vartheta > \varepsilon'(\varepsilon - \frac{\varepsilon'}{2})$$
$$\varepsilon \leq \varepsilon' < 2\gamma$$

e2] $0 < \rho_2 < \rho_1 < 1 < \Psi$

The necessary and sufficient conditions for $0<\rho_2<\rho_1<\Psi$ are (A115)-(A118).

The necessary and sufficient conditions for 1 to be greater than ρ_1, ρ_2 and less than Ψ are according to theorem A3,

$$\gamma\phi(1) > 0\ ,\quad 1 > (\rho_1 + \rho_2)/2\ ,\quad \varepsilon' > 2\gamma$$

Using (A11), (A1),

$$(\gamma - \varepsilon + \vartheta) > 0$$
$$1 > \varepsilon/2\gamma$$
$$\varepsilon' > 2\gamma$$

In summary, the necessary and sufficient conditions for tha arrangement $0 < \rho_2 < \rho_1 < 1 < \Psi$ are,

$$\varepsilon'^2 = 4\gamma\vartheta'$$
$$\varepsilon^2 - 4\gamma\vartheta > 0$$
$$2\gamma\vartheta > \varepsilon'(\varepsilon - \frac{\varepsilon'}{2})$$
$$\sup\{(\varepsilon - \vartheta),\ \varepsilon/2\} < \gamma < \varepsilon'/2$$

e3] $0 < \rho_2 < 1 < \rho_1 < \Psi$

The necessary and sufficient conditions for $0<\rho_2<\rho_1<\Psi$ are (A115)-(A118).

The necessary and sufficient conditions for 1 to lie between ρ_1 , ρ_2 are according to theorem A5,

$$\gamma\phi(1) < 0$$

Using (A11),

$$(\gamma - \varepsilon + \vartheta) < 0$$

In summary, the necessary and sufficient conditions for the arrangement $0 < \rho_2 < 1 < \rho_1 < \Psi$ are,

$$\varepsilon'^2 = 4\gamma\vartheta'$$
$$\varepsilon^2 - 4\gamma\vartheta > 0$$
$$2\gamma\vartheta > \varepsilon'(\varepsilon - \frac{\varepsilon'}{2})$$
$$\varepsilon' > \varepsilon$$
$$(\gamma - \varepsilon + \vartheta) < 0$$

e4] $1 < \rho_2 < \rho_1 < \Psi$

The necessary and sufficient conditions for $\rho_2 < \rho_1 < \Psi$ are (A115)-(A118).

The necessary and sufficient conditions for 1 to be less than ρ_1 , ρ_2 are according to theorem A1,

$$\gamma\phi(1) > 0 \, , \quad 1 < (\rho_1 + \rho_2)/2$$

Using (A11), (A1),

$$(\gamma - \varepsilon + \vartheta) > 0$$
$$1 < \varepsilon/2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $0 < \rho_2 < 1 < \rho_1 < \Psi$ are,

$$\varepsilon'^2 = 4\gamma\vartheta'$$
$$\varepsilon^2 - 4\gamma\vartheta > 0$$

$$2\gamma\vartheta > \varepsilon'(\varepsilon - \frac{\varepsilon'}{2})$$
$$2\gamma < \varepsilon < \varepsilon'$$
$$(\gamma - \varepsilon + \vartheta) > 0$$

f1] $0 < \rho_2 < \Psi < \rho_1 < 1$

The necessary and sufficient conditions for $0 < \rho_2 < \Psi < \rho_1$, where Ψ is a double root of $G(\omega) = 0$, are according to theorem A5,

$$\varepsilon'^2 = 4\gamma\vartheta'$$
$$\gamma\Phi(\varepsilon'/2\gamma) < 0$$

Using (A15),

$$\varepsilon'^2 = 4\gamma\vartheta' \qquad \text{(A119)}$$

$$2\gamma\vartheta < \varepsilon'(\varepsilon - \frac{\varepsilon'}{2}) \qquad \text{(A120)}$$

The necessary and sufficient conditions for 1 to be greater than ρ_1, ρ_2 are according to theorem A3,

$$\Delta_\phi > 0 \qquad \text{(A121)}$$

$$\gamma\Phi(1) > 0 \qquad \text{(A122)}$$

$$1 > (\rho_1 + \rho_2)/2 \qquad \text{(A123)}$$

Condition (A121) is repetitious, because according to theorem A5, the condition $\gamma\Phi(\varepsilon'/2\gamma) < 0$ guarantees that ρ_1, ρ_2 are real and unequal. Therefore, we can disregard (A121), and using (A11), (A1), we can write (A122)-(A123) as

$$(\gamma-\varepsilon+\vartheta)>0$$
$$1>\varepsilon/2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $0<\rho_2<\psi<\rho_1<1$ are,

$$\varepsilon'^2=4\gamma\vartheta'$$
$$2\gamma\vartheta<\varepsilon'(\varepsilon-\frac{\varepsilon'}{2})$$
$$(\gamma-\varepsilon+\vartheta)>0$$
$$\varepsilon<2\gamma$$

Or in a more compact form,

$$\varepsilon'^2=4\gamma\vartheta'$$
$$2\gamma\vartheta<\varepsilon'(\varepsilon-\frac{\varepsilon'}{2})$$
$$\gamma>\sup\{\varepsilon/2,(\varepsilon-\vartheta)\}$$

f2] $0<\rho_2<\psi<1<\rho_1$

The necessary and sufficient conditions for $0<\rho_2<\psi<\rho_1$ are (A119)-(A120).

The necessary and sufficient conditions for 1 to be between ρ_1, ρ_2 and greater than Ψ, are according to theorem A5,

$$\gamma\phi(1)<0,\quad \varepsilon'<2\gamma$$

Using (A11),

$$(\gamma-\varepsilon+\vartheta)<0$$
$$\varepsilon'<2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $0<\rho_2<\psi<1<\rho_1$ are,

$$\varepsilon'^2 = 4\gamma\vartheta'$$
$$2\gamma\vartheta < \varepsilon'\left(\varepsilon - \frac{\varepsilon'}{2}\right)$$
$$\frac{\varepsilon'}{2} < \gamma < (\varepsilon - \vartheta)$$

f3] $0 < \rho_2 < 1 < \Psi < \rho_1$

The necessary and sufficient conditions for $0 < \rho_2 < \Psi < \rho_1$ are (A119)-(A120).

The necessary and sufficient conditions for 1 to be between ρ_1, ρ_2 and less than Ψ, are according to theorem A5,

$$(\gamma - \varepsilon + \vartheta) < 0$$
$$\varepsilon' > 2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $0 < \rho_2 < 1 < \Psi < \rho_1$ are,

$$\varepsilon'^2 = 4\gamma\vartheta'$$
$$2\gamma\vartheta < \varepsilon'\left(\varepsilon - \frac{\varepsilon'}{2}\right)$$
$$\gamma < \inf\{\varepsilon'/2, (\varepsilon - \vartheta)\}$$

f4] $1 < \rho_2 < \Psi < \rho_1$

The necessary and sufficient conditions for $\rho_2 < \Psi < \rho_1$ are (A119)-(A120).

The necessary and sufficient conditions for 1 to be less than ρ_1, ρ_2 are according to theorem A1,

$$\gamma\Phi(1) > 0 \quad , \quad 1 < (\rho_1 + \rho_2)/2$$

Using (A11), (A1),

$$(\gamma - \varepsilon + \vartheta) > 0$$
$$1 < \varepsilon/2\gamma$$

In summary, the necessary and sufficient conditions for the arrangement $1 < \rho_2 < \Psi < \rho_1$ are,

$$\varepsilon'^2 = 4\gamma\vartheta'$$
$$2\gamma\vartheta < \varepsilon'\left(\varepsilon - \frac{\varepsilon'}{2}\right)$$
$$(\varepsilon - \vartheta) < \gamma < \varepsilon/2$$

g1] $0 < \rho < \Psi < 1$

g2] $0 < \rho < 1 < \Psi$

g3] $1 < \rho < \Psi$

h1] $0 < \Psi < \rho < 1$

h2] $0 < \Psi < 1 < \rho$

h3] $1 < \Psi < \rho$

i1] $0 < \rho = \Psi < 1$

i2] $1 < \rho = \Psi$

The necessary and sufficient conditions for the above arrangements are shown in chapter IVb. The derivation of these conditions is trivial, and will not be discussed.

CASE C

a1] ρ_1, ρ_2 are complex and $0 < \Psi_2 < \Psi_1 < 1$

The necessary and sufficient conditions for ρ_1, ρ_2 to be complex and for $0 < \Psi_2 < \Psi_1 < 1$ are according to theorem A4,

$$\varepsilon^2 < 4\gamma\vartheta$$
$$\varepsilon'^2 - 4\gamma\vartheta' > 0$$
$$-\gamma G(1) > 0$$
$$1 > (\Psi_1 + \Psi_2)/2$$

Using (A13), (A3),

$$\varepsilon^2 < 4\gamma\vartheta$$
$$\varepsilon'^2 - 4\gamma\vartheta' > 0$$
$$(\gamma - \varepsilon' + \vartheta') > 0$$
$$1 > \varepsilon'/2\gamma$$

Or in a more compact form,

$$\varepsilon^2 < 4\gamma\vartheta$$
$$\varepsilon'^2 - 4\gamma\vartheta' > 0$$
$$\gamma > \sup\{\varepsilon'/2, (\varepsilon' - \vartheta')\}$$

a2] ρ_1, ρ_2 are complex and $0 < \Psi_2 < 1 < \Psi_1$

The necessary and sufficient conditions for ρ_1, ρ_2 to be complex and for $0 < \Psi_2 < 1 < \Psi_1$ are according to theorem A6,

$$\varepsilon^2 - 4\gamma\vartheta < 0$$
$$-\gamma G(1) < 0$$

Using (A13),
$$\varepsilon^2 < 4\gamma\vartheta$$
$$(\gamma - \varepsilon' + \vartheta') < 0$$

a3] ρ_1 , ρ_2 are complex and $1 < \Psi_2 < \Psi_1$.

The necessary and sufficient conditions for ρ_1 , ρ_2 to be complex and for $1 < \Psi_2 < \Psi_1$ are according to theorem A2,
$$\varepsilon^2 - 4\gamma\vartheta < 0$$
$$\varepsilon'^2 - 4\gamma\vartheta' > 0$$
$$-\gamma G(1) > 0$$
$$1 < (\Psi_1 + \Psi_2)/2$$

Using (A13), (A3),
$$\varepsilon^2 - 4\gamma\vartheta < 0$$
$$\varepsilon'^2 - 4\gamma\vartheta' > 0$$
$$(\gamma - \varepsilon' + \vartheta') > 0$$
$$1 < \varepsilon'/2\gamma$$

Or in a more compact form,
$$\varepsilon^2 < 4\gamma\vartheta$$
$$\varepsilon'^2 > 4\gamma\vartheta'$$
$$(\varepsilon' - \vartheta') < \gamma < \varepsilon'/2$$

b1] ρ_1 , ρ_2 are complex and $0 < \psi < 1$

b2] ρ_1 , ρ_2 are complex and $1 < \psi$

The necessary and sufficient conditions for these arrangements are shown in chapter IVb. Their derivation is trivial and will not be discussed.

c1] ψ_1, ψ_2 are complex and $0 < \rho_2 < \rho_1 < 1$.

The necessary and sufficient conditions for ψ_1, ψ_2 to be complex and for $0 < \rho_2 < \rho_1 < 1$ are according to theorem A3,

$$\begin{gathered} \varepsilon'^2 - 4\gamma\vartheta' < 0 \\ \varepsilon^2 - 4\gamma\vartheta > 0 \\ \gamma\phi(1) > 0 \\ 1 > (\rho_1 + \rho_2)/2 \end{gathered}$$

Using (A11),(A1), we can write these conditions as

$$\begin{gathered} \varepsilon'^2 < 4\gamma\vartheta' \\ \varepsilon^2 > 4\gamma\vartheta \\ (\gamma - \varepsilon + \vartheta) > 0 \\ 1 > \varepsilon/2\gamma \end{gathered}$$

Or in a more compact form,

$$\begin{gathered} \varepsilon'^2 < 4\gamma\vartheta' \\ \varepsilon^2 > 4\gamma\vartheta \\ \gamma > \sup\{\varepsilon/2, (\varepsilon - \vartheta)\} \end{gathered}$$

c2] ψ_1, ψ_2 are complex and $0 < \rho_2 < 1 < \rho_1$

The necessary and sufficient conditions for ψ_1, ψ_2 to be complex and for $0 < \rho_2 < 1 < \rho_1$ are according to theorem A5,

$$\begin{gathered} \varepsilon'^2 - 4\gamma\vartheta' < 0 \\ \gamma\phi(1) < 0 \end{gathered}$$

Using (A11),

$$\begin{gathered} \varepsilon'^2 < 4\gamma\vartheta' \\ (\gamma - \varepsilon + \vartheta) < 0 \end{gathered}$$

c3] Ψ_1, Ψ_2 are complex and $1 < \rho_2 < \rho_1$.

The necessary and sufficient conditions for Ψ_1, Ψ_2 to be complex and for $1 < \rho_2 < \rho_1$ are according to theorem A1,

$$\begin{gathered} \varepsilon'^2 - 4\gamma\vartheta' < 0 \\ \varepsilon^2 - 4\gamma\vartheta > 0 \\ \gamma\Phi(1) > 0 \\ 1 < (\rho_1 + \rho_2)/2 \end{gathered}$$

Using (A11), (A1),

$$\begin{gathered} \varepsilon'^2 < 4\gamma\vartheta' \\ \varepsilon^2 > 4\gamma\vartheta \\ (\gamma - \varepsilon + \vartheta) > 0 \\ 1 < \varepsilon/2\gamma \end{gathered}$$

Or in a more compact form,

$$\begin{gathered} \varepsilon'^2 < 4\gamma\vartheta' \\ \varepsilon^2 > 4\gamma\vartheta \\ (\varepsilon - \vartheta) < \gamma < \frac{\varepsilon}{2} \end{gathered}$$

d1] Ψ_1, Ψ_2 are complex and $0 < \rho < 1$

d2] Ψ_1, Ψ_2 are complex and $1 < \rho$

e] Ψ_1, Ψ_2 and ρ_1, ρ_2 are complex.

The necessary and sufficient conditions for the above arrangements are shown in chapter IVb. Their derivation is trivial and will not be discussed.

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Nomenclature

English characters

a_0 : Constant defined in chapter VI.

a_1 : " " " " "

a_2 : " " " "

a_3 : " " " "

a_0' : " " " "

a_1' : " " " "

a_2' : " " " "

a_3' : " " " "

A : Reactant

[A] : Concentration of A

$\underline{A}$: Linearized matrix defined in IIIa.

(A-S) : Adsorbed reactant A.

{A-S} : Number of active sites occupied by adsorbed A.

B : Reactant

[B] : Concentration of B.

(B-S) : Adsorbed reactant B.

{B-S} : Number of active sites occupied by adsorbed B.

E_3 : Activation energy of adsorption. Defined in IIb.

f : Function defined in VI.

f_1 : Function defined in IIc.

f_2 : " " " "

F	:	Function defined in VI.
G	:	Polynomial defined in IIIc.
k	:	Kinetic constant defined in IIb.
k_1	:	Kinetic constant for adsorption of A(g).
k_2	:	" " " " " B(g).
k_{-1}	:	Kinetic constant for desorption of (A-S).
k_{-2}	:	" " " " " (B-S).
k_3	:	Rate constant defined in IIb.
k_{30}	:	Kinetic constant comprising k_3.
k_3^0	:	= kL
k_2'	:	Kinetic constant for Eley-Rideal surface mechanism
L	:	Total number of active surface sites.
m	:	Real number(see APPENDIX).
M	:	" " "
r	:	Reaction rate defined in IIb.
R	:	Universal gas constant
$R_{G\Phi}$	:	Constant defined in the APPENDIX, page 91.
[S]	:	Active surface site.
{S}	:	Number of active sites which are not occupied at time t.
T	:	Temperature
t	:	Time
x	:	Coverage of catalytic surface with adsorbed A(g).
y	:	" " " " " " B(g).
$\underline{Y}$	:	Vector defined in IIIa
Z	:	Polynomial defined in VI.

Greek characters

$\alpha_1, \alpha_2, \alpha_3, \beta$: Constants defined in IIIa

β_1, β_2 : Constants defined in IId

γ : " " " IIIc.

δ : " " " VI

Δ_ϕ, Δ_G : " " " IIId

$\varepsilon, \varepsilon'$: " " " IIIc

ζ : Fraction of active sites left unoccupied at time t.

$\vartheta, \vartheta', \Theta$: Constants defined in IIIc

λ_1, λ_2 : Eigenvalues of linearized matrix $\underline{A}$

μ : Coefficient of heterogeneity of catalytic surface.

ξ : Unknown in equation $\phi(\xi)=0$.

ρ_1, ρ_2 : Roots of equ. $\phi(\xi)=0$, defined in IIId.

ρ : Double root of $\phi(\xi)=0$, $=\varepsilon/2\gamma$.

τ : $=k_3^0$

ϕ : Polynomial defined in IIIc

ψ_1, ψ_2 : Roots of equ. $G(\omega)=0$, defined in IIId.

ψ : Double root of equ. $G(\omega)=0$, $=\varepsilon'/2\gamma$.

ω : Unknown in equ. $G(\omega)=0$.

Ω : Polynomial defined in VI.

Symbols in Script

$\mathcal{H}$: Constant defined in IIIa.