Exercise Set 5

Problem 1

The equilibrium points are given by the following curves in the (μ, u) plane (see figure below):

$$\begin{aligned} u &= 0 \\ 9 - \mu u &= 0 \\ \mu + 2u - u^2 &= 0 \end{aligned}$$

At $(\mu, u) = (-1, 1)$, $\frac{d\mu}{du}$ changes sign. We have

$$f_\mu(\mu, u) = u(9 - 2u\mu - 2u^2 + u^3)$$

Hence $f_\mu(-1, 1) = 10 \neq 0$ and $(-1, 1)$ is a regular turning point where stability is exchanged.

We differentiate f_μ once more and get

$$f_{\mu\mu} = -2u^2$$

At (μ_1, u_1), the intersection between the two curves $9 - \mu u = 0$ and $\mu + 2u - u^2 = 0$, $f_u = 0$ but $f_{\mu\mu}$ does not vanish. Thus, we have a double point and stability is exchanged (theorem 2.4, p.370 in Logan).

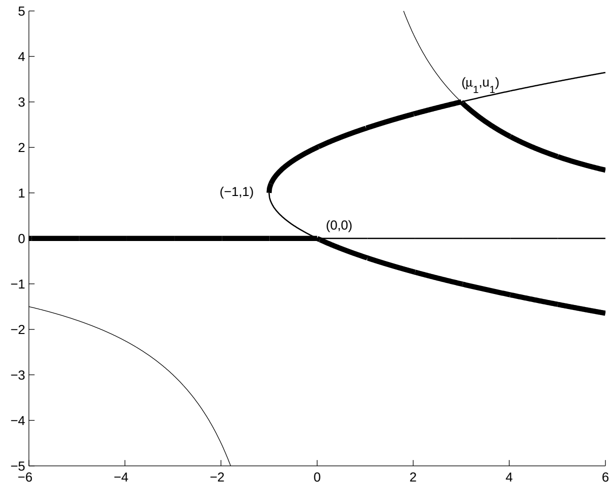
$f_{\mu\mu}(0, 0) = 0$ but $f_{\mu u}(0, 0) = 9 \neq 0$. $(0, 0)$ is a double point and stability is also exchanged (theorem 2.5, p.371 in Logan).

It then suffices to compute the sign of f_u at one point of each curve to determine the stability along all the curves. We have

$$f_u = (9 - \mu u)(\mu + 2u - u^2) - \mu u(\mu + 2u - u^2) + u(9 - \mu u)(-2u + 2)$$

We choose for example (μ, u) equal to $(0, 2)$, $(0, -\infty)$, $(\mu, \frac{9}{\mu})$ $\mu \to \infty$. We get

$$\begin{aligned} f_u(0, 2) &= -180 \\ \lim_{\mu \to -\infty} f_u(0, u) &= -\infty \\ \lim_{u \to \infty} f_u(\mu, 9\frac{9}{\mu}) &= -\infty \end{aligned}$$



The thick lines indicate stable equilibrium points

Problem 2

The infinitesimal change ds^* due to the chemical reaction is as in the textbook

$$ds^* = (-k_1 s^* e^* + k_{-1} c^*)dt^* \tag{1}$$

The infinitesimal change due to the reactor is

$$\begin{aligned} ds^* &= d(\frac{m_s}{V_R}) \\ &= \frac{1}{V_R} dm_s \end{aligned}$$

where m_s is the mass of substract in the reactor. Since

$$dm_s = V s_0 dt^* - V s^* dt \ ,$$

we get

$$ds^* = \frac{V}{V_R}(s_0 - s^*)dt^* \tag{2}$$

We add up the two contributions (1) and (2) and get

$$\frac{ds^*}{dt^*} = -k_1 s^* e^* + k_{-1} c^* + \frac{V}{V_R}(s_0 - s^*)$$

We proceed in the same way for the remaining variables c^*, e^*, p^* and get the following system of o.d.e :

$$\frac{ds^*}{dt^*} = -k_1 s^* e^* + k_{-1} c^* + \frac{V}{V_R}(s_0 - s^*) \tag{3}$$
$$\frac{dc^*}{dt^*} = k_1 s^* e^* - k_{-1} c^* - k_2 c^* - \frac{V}{V_R} c^* \tag{4}$$
$$\frac{de^*}{dt^*} = -k_1 s^* e^* + k_{-1} c^* + k_2 c^* + \frac{V}{V_R}(e_0 - e^*) \tag{5}$$
$$\frac{dp^*}{dt^*} = k_2 c^* - \frac{V}{V_R} p^* \tag{6}$$

Summing equations (3), (4) and (6), we obtain

$$\frac{d}{dt^*}(s^* + c^* + p^*) = \frac{V}{V_R} s_0 - \frac{V}{V_R}(s^* + c^* + p^*)$$

and, similarly with (4) and (5),

$$\frac{d}{dt^*}(c^* + e^*) = \frac{V}{V_R} e_0 - \frac{V}{V_R}(c^* + e^*)$$

We set

$$f^* = c^* + e^* \quad \text{and} \quad g^* = s^* + c^* + p^* \tag{7}$$

The previous system of ode is then equivalent to

$$\frac{ds^*}{dt^*} = -k_1 s^* (f^* - c^*) + k_{-1} c^* + \frac{V}{V_R}(s_0 - s^*)$$
$$\frac{dc^*}{dt^*} = k_1 s^* (f^* - c^*) - k_{-1} c^* - k_2 c^* - \frac{V}{V_R} c^*$$
$$\frac{df^*}{dt^*} = \frac{V}{V_R}(e_0 - f^*)$$
$$\frac{dg^*}{dt^*} = \frac{V}{V_R}(s_0 - g^*)$$

We rescale the problem

$$s^* = s_0 s \qquad c^* = e_0 c \qquad f^* = e_0 f$$
$$g^* = s_0 g \qquad t^* = \frac{t}{k_1 e_0}$$

and set

$$\kappa = \frac{k_{-1} + k_2}{k_1 s_0} \qquad \lambda = \frac{k_2}{k_1 s_0}$$
$$\varepsilon = \frac{e_0}{s_0} \qquad \mu = \frac{V}{V_R k_1 e_0}$$

We end up with the following equivalent but simpler system of ode

$$\begin{aligned}
\dot{s} &= -fs + (s + \kappa - \lambda)c + \mu(1 - s) \\
\varepsilon\dot{c} &= fs - (s + \kappa)c - \varepsilon\mu c \\
\dot{f} &= \mu(1 - f) \\
\dot{g} &= \mu(1 - g)
\end{aligned}$$

The equilibrium points ($\dot{s} = \dot{c} = \dot{f} = \dot{g} = 0$) satisfy

$$\begin{aligned}
f &= 1 \\
g &= 1
\end{aligned}$$

and

$$-s + (s + \kappa - \lambda)c + \mu(1 - s) = 0 \tag{8}$$

$$s - (s + \kappa)c - \varepsilon\mu c = 0 \tag{9}$$

Adding up these two equations, we get

$$(\lambda + \varepsilon\mu)c + \mu s = \mu \tag{10}$$

We use equation (10) to express s in function of c and plug the result into equation (9). We get

$$F(c) \equiv (\mu - (\lambda + \varepsilon\mu)c)(1 - c) - (\kappa + \varepsilon\mu)\mu c = 0$$

$F(c)$ is a quadratic polynomial. $F(0) = \mu > 0$ and $F(1) = -\mu(\kappa+\varepsilon\mu) < 0$ imply that there exists $c_* \in (0, 1)$ such that $F(c_*) = 0$. F has an other root in $(1, \infty)$ because $\lim_{c\to\infty} F(c) = +\infty$ but this root cannot give a equilibrium point since $1 = c + e$ (at equilibrium) implies that $c \leq 1$ (e is positive). Therefore, if we have an equilibrium point, we must have $c = c_*$.

Once c_* is known, the value of s at equilibrium (which we denote s_*) is given by (10) and p_* and e_* (the values of p and e at equilibrium) by (7). We have to check if these values are admissible i.e. if they are positive (concentrations must be positive). In dimensionless variables, equation (7) yields

$$f_* = 1 = c_* + e_* \quad \text{and} \quad g_* = 1 = s_* + \varepsilon c_* + p_*$$

Since $c_* \in (0, 1)$, $e_* \geq 0$. It remains to check that $s_* \geq 0$ and $s_* + \varepsilon c_* \leq 1$ so that $p_* \geq 0$. (9) implies

$$s_* = \frac{(\varepsilon\mu + \kappa)c_*}{1 - c}$$

and since $c \in (0, 1)$, $s_* \geq 0$. (10) gives

$$\varepsilon c_* + s_* = 1 - \frac{\lambda}{\mu}$$

and therefore $\varepsilon c_* + s_* \leq 1$.

We have then proved that there exists an admissible equilibrium point and that it is unique. We now investigate the stability of this equilibrium point. We write down the matrix corresponding to the linearized system at $(s_*, c_*, f_* = 1, g_* = 1)$

$$M = \begin{pmatrix} -1 + c_* - \mu & s_* + \kappa - \lambda & -s_* & 0 \\ \dfrac{1 - c*}{\varepsilon} & \dfrac{-(s_* + \kappa_*) - \varepsilon\mu}{\varepsilon} & \dfrac{s_*}{\varepsilon} & 0 \\ 0 & 0 & -\mu & 0 \\ 0 & 0 & 0 & -\mu \end{pmatrix}$$

The eigenvalues of M are given by the roots of $det[M - \lambda I]$. We have

$$det[M - \lambda I] = (-\mu - \lambda)^2 det[\tilde{M} - \lambda I]$$

where

$$\tilde{M} = \begin{pmatrix} -1 + c_* - \mu & s_* + \kappa - \lambda \\ \dfrac{1 - c_*}{\varepsilon} & \dfrac{-(s_* + \kappa) - \varepsilon\mu}{\varepsilon} \end{pmatrix}.$$

$-\mu$ is a double eigenvalue. The two remaining eigenvalues of M are the same as those of $\tilde{M}$. The product of the eigenvalues of a 2x2 matrix is equal to the determinant of the matrix while the sum is equal to the trace. We have

$$det\tilde{M} = \frac{1}{\varepsilon}\left[(\varepsilon\mu + \lambda)(1 - c_*) + \mu(s_* + \kappa + \varepsilon\mu)\right] > 0$$

and

$$tr\tilde{M} = -(1 - c_*) - 2\mu - \frac{s_* + \kappa}{\varepsilon}$$

If λ_1 and λ_2, the eigenvalues of $\tilde{M}$, are real, $\lambda_1\lambda_2 > 0$ implies that λ_1 and λ_2 have the same sign but, since $\lambda_1 + \lambda_2 < 0$, they can only be strictly negative.

If λ_1 and λ_2 are imaginary, they must be conjugate: $\lambda_2 = \overline{\lambda_1}$. $\lambda_1 + \lambda_2 < 0$ implies $\lambda_1 + \overline{\lambda_1} < 0$. Hence,

$$Re[\lambda_1] = Re[\lambda_2] < 0$$

In both cases, we have a stable equilibrium point.