Linearization

Here are two different ways of looking at linearization. Both methodologies are correct and this file serves to give you, the student, the option to choose what suits you best.

1 As seen in class

1.1 Linearization procedure around a stationary point

Once, you have a nonlinear model, you have to linearize it to be able to work with it. A linear approximation for a function $f(x)$ around $\bar{x}$ looks like

$$f(\bar{x}+\delta f) \approx f(\bar{x}) + \frac{df(\bar{x})}{dx}\delta x = f(\bar{x}) + \delta f. \tag{1}$$

For a general problem,

$$\begin{aligned}\frac{dx}{dt} &= f(x(t),u(t)),\\ y(t) &= g(x(t),u(t)),\\ x(0) &= x_0.\end{aligned}$$

The linearized system around $\bar{x}$ then looks like

$$\begin{aligned}\frac{dx}{dt} &= f(\bar{x},\bar{u}) + \left.\frac{\partial f}{\partial x}\right|_{\bar{x},\bar{u}}(x-\bar{x}) + \left.\frac{\partial f}{\partial u}\right|_{\bar{x},\bar{u}}(u-\bar{u}),\\ y(t) &= g(\bar{x},\bar{u}) + \left.\frac{\partial g}{\partial x}\right|_{\bar{x},\bar{u}}(x-\bar{x}) + \left.\frac{\partial g}{\partial u}\right|_{\bar{x},\bar{u}}(u-\bar{u}),\\ x(0) &= x_0.\end{aligned}$$

Now define the deviations

$$\begin{aligned}\delta x(t) &= x(t)-\bar{x},\\ \delta u(t) &= u(t)-\bar{u},\\ \delta y(t) &= y(t)-\bar{y}.\end{aligned}$$

The linear approximation then becomes

$$\begin{aligned}\frac{d\delta x}{dt} &= \left.\frac{\partial f}{\partial x}\right|_{\bar{x},\bar{u}}\delta x + \left.\frac{\partial f}{\partial u}\right|_{\bar{x},\bar{u}}\delta u,\\ \delta y(t) &= \left.\frac{\partial g}{\partial x}\right|_{\bar{x},\bar{u}}\delta x + \left.\frac{\partial g}{\partial u}\right|_{\bar{x},\bar{u}}\delta u,\\ \delta x(0) &= x_0-\bar{x}.\end{aligned}$$

These equations can be generalized for systems of equations. A system has the form

$$\begin{aligned}\frac{d\delta\mathbf{x}(t)}{dt} &= A\delta\mathbf{x}(t) + B\delta\mathbf{u}(t)\\ \delta\mathbf{y}(t) &= C\delta\mathbf{x}(t) + D\delta\mathbf{u}(t),\\ \delta\mathbf{x}(0) &= \mathbf{x}_0-\bar{\mathbf{x}}.\end{aligned}$$

The matrices in these equations are constructed by using the same logic as the single equation logic. Namely,

$$A = \left.\frac{\partial f}{\partial x}\right|_{\bar{\mathbf{x}},\bar{\mathbf{u}}} = \left.\begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \cdots & \frac{\partial f_n}{\partial x_n} \end{bmatrix}\right|_{\bar{\mathbf{x}},\bar{\mathbf{u}}},$$

$$B = \left.\frac{\partial f}{\partial u}\right|_{\bar{\mathbf{x}},\bar{\mathbf{u}}} = \left.\begin{bmatrix} \frac{\partial f_1}{\partial u_1} & \frac{\partial f_1}{\partial u_2} & \cdots & \frac{\partial f_1}{\partial u_p} \\ \frac{\partial f_2}{\partial u_1} & \frac{\partial f_2}{\partial u_2} & \cdots & \frac{\partial f_2}{\partial u_p} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial u_1} & \frac{\partial f_n}{\partial u_2} & \cdots & \frac{\partial f_n}{\partial u_p} \end{bmatrix}\right|_{\bar{\mathbf{x}},\bar{\mathbf{u}}}$$

$$C = \left.\frac{\partial g}{\partial x}\right|_{\bar{\mathbf{x}},\bar{\mathbf{u}}} = \left.\begin{bmatrix} \frac{\partial g_1}{\partial x_1} & \frac{\partial g_1}{\partial x_2} & \cdots & \frac{\partial g_1}{\partial x_n} \\ \frac{\partial g_2}{\partial x_1} & \frac{\partial g_2}{\partial x_2} & \cdots & \frac{\partial g_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial g_q}{\partial x_1} & \frac{\partial g_q}{\partial x_2} & \cdots & \frac{\partial g_q}{\partial x_n} \end{bmatrix}\right|_{\bar{\mathbf{x}},\bar{\mathbf{u}}}$$

$$D = \left.\frac{\partial g}{\partial u}\right|_{\bar{\mathbf{x}},\bar{\mathbf{u}}} = \left.\begin{bmatrix} \frac{\partial g_1}{\partial u_1} & \frac{\partial g_1}{\partial u_2} & \cdots & \frac{\partial g_1}{\partial u_p} \\ \frac{\partial g_2}{\partial u_1} & \frac{\partial g_2}{\partial u_2} & \cdots & \frac{\partial g_2}{\partial u_p} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial g_q}{\partial u_1} & \frac{\partial g_q}{\partial u_2} & \cdots & \frac{\partial g_q}{\partial u_p} \end{bmatrix}\right|_{\bar{\mathbf{x}},\bar{\mathbf{u}}}$$

1.2 Toy example

Given the system

$$\frac{dx(t)}{dt} = -2x + 0.5(x+1)u, \qquad x(0) = 1,$$

linearize it around the equilibrium point.

Solution
Firstly, lets determine the equilibrium point. That is defined as

$$\frac{dx(t)}{dt} = 0.$$

Hence,

$$\begin{aligned} \bar{x} &= 1, \\ \bar{u} &= 2. \end{aligned}$$

The approximation of the nonlinearity in this case is

$$xu \simeq \bar{x}\bar{u} + \bar{u}(x - \bar{x}) + \bar{x}(u - \bar{u}) \tag{2}$$

The linear approximation of the whole system then becomes

$$\begin{aligned} \frac{dx(t)}{dt} &= (-2x + 0.5(\bar{x}\bar{u} + \bar{u}\delta x + \bar{x}\delta u) + 0.5u) - (-2\bar{x} + 0.5\bar{x}\bar{u} + 0.5\bar{u}) \\ &= -2\delta x + 0.5(\bar{u}\delta x + \bar{x}\delta u) + 0.5\delta u \\ \frac{d\delta x(t)}{dt} &= -2\delta x + 0.5(\bar{u}\delta x + \bar{x}\delta u) + 0.5\delta u \end{aligned}$$

Filling in the numerical values of $\bar{x} = 1, \bar{u} = 2$, gives the final result

$$\frac{d\delta x(t)}{dt} = -\delta x + \delta u, \qquad \delta x(0) = 0 \tag{3}$$

2 A systematic way

2.1 Why linearization and how to do it?

In general, life is not linear and models are rarely linear naturally as a result. However, non-linearities make mathematics extremely difficult especially when systems of equations are being considered. Most of the mathematics in this course are for linear systems, hence we would like to *make* a system linear. A way of doing that is using a Taylor expansion around an arbitrary point. For a general function $f(x)$ around point a, it becomes

$$f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \cdots \tag{4}$$

Now, this is still not linear. Let's say that we do not want to describe a whole function, but only a point very close to a. For only a very small deviation from a, meaning $x-a$ small, higher order terms will approximate zero. Hence,

$$f(x) \simeq f(a) + \frac{f'(a)}{1!}(x-a) \tag{5}$$

Using this approximations, we can transform general differential equations into linear differential equations.

Finally, we can generalize this by looking at multivariate functions. Let's say for a function $F(x_1, x_2, \ldots, x_N)$. A linearization around $\mathbf{a} = [\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_N]$, looks like

$$F(x_1, x_2, \ldots, x_N) \simeq F(\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_N) + \sum_{i=1}^{N}\left(\left.\frac{\partial F}{\partial x_i}\right|_{\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_N}(x_i - \bar{x}_i)\right)$$

2.2 Small sidestep: Writing balances and notation

In this course, you will have to write balances very regularly. **I highly recommend writing a balance in a conceptual way before plugging in math even if it is in a different format than what I provide here.** We assume that you have seen this, but just to avoid confusion, I will explain here how I write these and how to fit things in. A classical balance for me looks like this

$$\text{(Accumulation)} = \text{(In)} - \text{(Out)} + \text{(Generation)} + \text{(Exchange)} \tag{6}$$

Herein, the *Generation* term signifies the creation or destruction of a species such as in a reaction. This term is 0 in non-reacting systems. The *Exchange* term is mostly seen in energy balances depending on how you define your system. It describes the flux of whatever the balance is about over the boundary of the system. An example is a cooling jacket on a reactor.

2.3 An example: A variation on Exercise 1 from Series 4

Description Consider a mixing tank with inlet volume flow rates q_1 and q_2 and with outlet flow rate $q_s(t) = k\sqrt{h(t)}$ where $h(t)$ represents the level of the liquid in the tank. Knowing that the densities (volumetric mass) of the liquids in the feed are equal and constant, linearize the system.

Solution

Let's start with a mass balance over the system. That gives

$$\text{(Accumulation)} = \text{(In)} - \text{(Out)} + \text{(Generation)} + \text{(Exchange)}, \tag{7}$$

$$\frac{dm}{dt} = \dot{m}_{in} - \dot{m}_{out} + 0 + 0, \tag{8}$$

$$\frac{d(\rho_V \cdot V)}{dt} = \rho_1 q_1 + \rho_2 q_2 - \rho_s q_s, \tag{9}$$

$$\frac{d(\rho_V \cdot S \cdot h(t))}{dt} = \rho_1 q_1 + \rho_2 q_2 - \rho_s k\sqrt{h(t)}. \tag{10}$$

This is the most general way of describing the problem. However, we can make some assumptions and also use additional information from the description. I will assume that the area of the vessel does not change $S \neq f(t)$. The densities of all flows are identical, hence the density in the vessel is constant, so $\rho_1 = \rho_2 = \rho s = \rho_V = \rho \neq f(t)$. The system then simplifies to

$$S\frac{dh(t)}{dt} = q_1 + q_2 - k\sqrt{h(t)}. \tag{11}$$

This is the non-linear description of the system. In a mathematically rigorous way, we can also write

$$\frac{dh(t)}{dt} = F(h, q_1, q_2), \tag{12}$$

$$F(q_1, q_2, h) = \frac{1}{S}(q_1 + q_2 - k\sqrt{h(t)}). \tag{13}$$

Let's say we linearize the system around an arbitrary point $\bar{h}, \bar{q_1}, \bar{q_2}$. First, let's define the deviations from this point as

$$\begin{aligned}\delta q_1 &= q_1 - \bar{q_1},\\ \delta q_2 &= q_2 - \bar{q_2},\\ \delta h &= h(t) - \bar{h}.\end{aligned}$$

Then the linearized system is

$$F(h, q_1, q_2) \simeq F(\bar{h}, \bar{q_1}, \bar{q_2}) + \left.\frac{\partial F(q_1, q_2, h)}{\partial q_1}\right|_{\bar{h},\bar{q_1},\bar{q_2}}(q_1 - \bar{q_1}) \tag{14}$$

$$+ \left.\frac{\partial F(q_1, q_2, h)}{\partial q_2}\right|_{\bar{h},\bar{q_1},\bar{q_2}}(q_2 - \bar{q_2}) + \left.\frac{\partial F(q_1, q_2, h)}{\partial h}\right|_{\bar{h},\bar{q_1},\bar{q_2}}(h(t) - \bar{h}) \tag{15}$$

Wherein,

$$\begin{aligned}\left.\frac{\partial F(q_1, q_2, h)}{\partial q_1}\right|_{\bar{h},\bar{q_1},\bar{q_2}}(q_1 - \bar{q_1}) &= \frac{1}{S}(q_1 - \bar{q_1})\\ \left.\frac{\partial F(q_1, q_2, h)}{\partial q_2}\right|_{\bar{h},\bar{q_1},\bar{q_2}}(q_2 - \bar{q_2}) &= \frac{1}{S}(q_2 - \bar{q_2})\\ \left.\frac{\partial F(q_1, q_2, h)}{\partial h}\right|_{\bar{h},\bar{q_1},\bar{q_2}}(h(t) - \bar{h}) &= \frac{-k}{2S\sqrt{\bar{h}}}(h(t) - \bar{h})\end{aligned}$$

Now, we can describe the system as a linear system. Namely,

$$\frac{d(\delta h)}{dt} = \frac{1}{S}(\delta q_1 + \delta q_2 - \frac{k}{2\sqrt{\bar{h}}}\delta h) \tag{16}$$

This is the solution of the problem. You might wonder where the term $F(\bar{h}, \bar{q_1}, \bar{q_2})$ went. In Eq. (16), we are looking at the change in the deviation of $h(t)$ from $\bar{h}$ with respect to time. That means that at $t = 0, h(t) = \bar{h}$, which means the deviation is zero at that point.

2.4 Old exam exercise

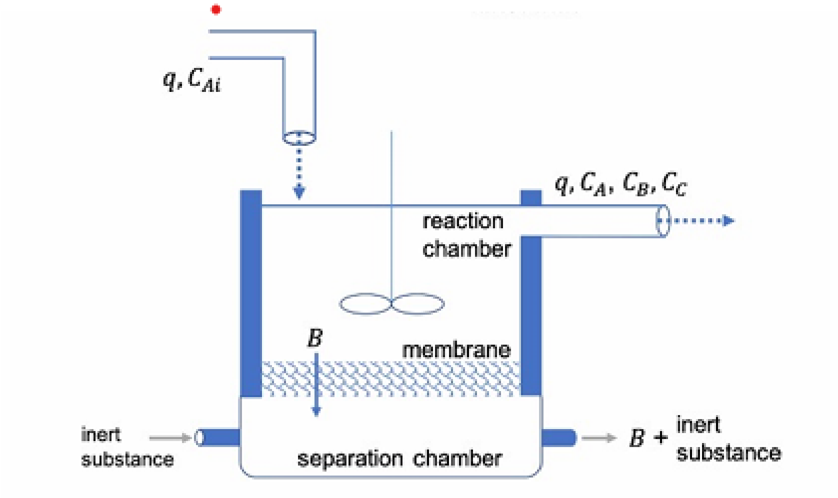
Problem statement (30 points) A reversible reaction $2A \rightleftharpoons B+C$ takes place in a membrane reactor shown below. The reactor consists of a well-mixed reaction chamber and a separation chamber separated by a membrane. The membrane is permeable to compound B, whereas compounds A and C cannot pass through. Compound B diffuses out of the reaction chamber through the membrane and is removed from the separation chamber by a stream of inert substance. The diffusion rate of B through the membrane is ($k_m A_m C_B \left[\frac{\text{kmol}}{\text{min}}\right]$), where ($A_m$) is the effective area of the membrane. Compound A is pumped into the reactor with the flow rate (q) and the concentration (C_{Ai}). (C_A, C_B, and C_C) denote the concentrations of A, B, and C in the reactor. Despite the diffusion of B through the membrane, the exit and feed flow rates are assumed equal because B is a small molecule, i.e., it is assumed that the reactor volume is constant. The temperature in the reactor is also constant. The reaction follows the mass action kinetics with the rate constants ($k_1 = 0.5\frac{m^3}{\text{kmol}\cdot\text{min}}$) (in the forward direction) and ($k_2 = 2.5\frac{m^3}{\text{kmol}\cdot\text{min}}$) (in the reverse direction).

For the parameter values: reactor volume ($V = 3\text{m}^3$), feed flow rate ($q = 0.25\text{m}^3/\text{min}$), mass transfer coefficient ($k_m = 1.5\text{m}/\text{min}$), and input feed concentration ($C_{Ai} = 10\text{kmol}/\text{m}^3$).

a) Write the mass balances for compounds A and B.

b) Knowing that the effective membrane area at the steady state is ($A_m^{SS} = 4, \text{m}^2$), and that the steady-state concentration of compound A is five times the one of B, i.e. ($C_A^{SS} = 5C_B^{SS}$), determine the steady-state concentrations of A, B, and C in the reaction chamber.

c) The membrane degrades gradually and its effective area, (A_m), changes in time. Derive the dynamic equations for deviations of concentrations (C_A) and (C_B) by linearizing the system of equations from (a) around the steady state derived in (b).



Question A

The mass balance for both A and B can be written as

$$(\text{Accumulation})_i = (\text{In})_i - (\text{Out})_i + (\text{Generation})_i + (\text{Exchange})_i. \tag{17}$$

Adapting this equation for species A, it becomes

$$\begin{aligned}
\frac{dm_A}{dt} &= \dot{m}_{A,in} - \dot{m}_{A,out} + \frac{1}{M_A} r_A V, \\
\frac{d(\rho_{A,V} \cdot V)}{dt} &= \rho_{A,in} q - \rho_A q + \frac{1}{M_A} r_A V \\
\frac{d(\frac{C_{A,V}}{M_A} \cdot V)}{dt} &= \frac{C_{A,in}}{M_A} q - \frac{C_A}{M_A} q + \frac{1}{M_A} r_A V
\end{aligned}$$

Herein, M_A the molar mass of A, a constant value. Furthermore, the vessel is well-mixed, so $C_{A,V} = C_A$, and I will assume that the reactor volume constant $V \neq f(t)$. Therefore,

$$V\frac{dC_A}{dt} = C_{A,in}q - C_Aq + r_AV. \tag{18}$$

Finally, since the kinetics are mass action. Then,

$$-\frac{1}{2}r_A = r_B = r_C = k_1C_A^2 - k_2C_BC_C$$

Filling that into the equation, yields the final mass balance for compound A.

$$V\frac{dC_A}{dt} = C_{A,in}q - C_Aq - 2V(k_1C_A^2 - k_2C_BC_C). \tag{19}$$

For compound B, only the first steps differ slightly. The initial equation is

$$\frac{dm_B}{dt} = 0 - \dot{m}_{B,out} + \frac{1}{M_B}r_BV + \dot{m}_{B,membrane}, \tag{20}$$

$$\frac{dm_B}{dt} = -\dot{m}_{B,out} - \frac{1}{M_B}r_BV - \frac{1}{M_B}k_mA_mC_B, \tag{21}$$

The reasoning is from this point identical to the reasoning of compound A. The final equation becomes

$$V\frac{dC_B}{dt} = C_Bq + V(k_1C_A^2 - k_2C_BC_C) - k_mA_mC_B. \tag{22}$$

Question B

At a steady state, the rates of change of the concentrations are 0. Hence, $\frac{dm_i}{dt} = o$ The mass balance for A becomes

$$\begin{aligned} 0 &= -\frac{q}{V}C_A^{SS} + \frac{q}{V}C_{Ai} - 2[(C_A^{SS})^2k_1 - k_2C_B^{SS}C_C], \\ \Rightarrow k_1(C_A^{SS})^2 - k_2C_B^{SS}C_C &= \frac{q}{2V}(C_{Ai} - C_A^{SS}). \end{aligned} \tag{B1}$$

Similarly, the mass balance for B becomes:

$$\begin{aligned} 0 &= -\frac{q}{V}C_B^{SS} + (C_A^{SS})^2k_1 - k_2C_B^{SS}C_C - \frac{K_mA_mC_B^{SS}}{V}, \\ \Rightarrow k_1(C_A^{SS})^2 - k_2C_B^{SS}C_C &= \frac{1}{V}(qC_B^{SS} + K_mA_mC_B^{SS}), \\ \Rightarrow k_1(C_A^{SS})^2 - k_2C_B^{SS}C_C &= \frac{1}{V}(q + K_mA_m)C_B^{SS}. \end{aligned} \tag{B2}$$

If we equate the left hand side of (B1) and (B2) and plug in the relationship that $C_A^{SS} = 5C_B^{SS}$, we get

$$\begin{aligned} \frac{1}{V}(q + K_mA_m)C_B^{SS} &= \frac{q}{2V}(C_{Ai} - 5C_B^{SS}), \\ \Rightarrow 2 * (0.25 + 1.5 * 4)C_B^{SS} &= 0.25(10 - 5C_B^{SS}), \\ \Rightarrow 2 * 6.25C_B^{SS} &= 2.5 - 1.25C_B^{SS}, \\ \Rightarrow 13.75C_B^{SS} &= 2.5, \\ \Rightarrow C_B^{SS} = \frac{2.5}{13.75}, \quad C_A^{SS} &= \frac{12.5}{13.75}. \end{aligned}$$

Plugging in these values into (B1), we get:

$$
\begin{aligned}
0.5 * \frac{12.5}{13.75} * \frac{12.5}{13.75} - \frac{2.5}{13.75} * C_C &= \frac{0.25}{2*3} * \left(10 - \frac{12.5}{13.75}\right), \\
\Rightarrow 12 * \frac{12.5}{13.75} * \frac{12.5}{13.75} - 60 * \frac{2.5}{13.75} * C_C &= \left(10 - \frac{12.5}{13.75}\right), \\
\Rightarrow 12 * \frac{156.25}{13.75^2} - \frac{150}{13.75} * C_C &= \frac{137.5 - 12.5}{13.75}, \\
\Rightarrow \frac{1875}{13.75} - \frac{150}{13.75} C_C &= \frac{125}{13.75}, \\
\Rightarrow 136.36 - 150 * C_C &= 125, \\
\Rightarrow C_C &= 0.07575.
\end{aligned}
$$

Question C
Let's explicitly write the mass balances with its dependencies on time.

$$
\frac{dC_A(t)}{dt} = \frac{1}{V}(C_{A,i}q - C_A(t))q - 2V(k_1(C_A(t))^2 - k_2 C_B(t) C_C(t))), \tag{23}
$$

$$
\frac{dC_B(t)}{dt} = \frac{1}{V}(C_B(t)q + V(k_1(C_A(t))^2 - k_2 C_B(t) C_C(t)) - k_m A_m(t) C_B(t)). \tag{24}
$$

Then,

$$
\begin{aligned}
\frac{dC_A(t)}{dt} &= F(C_A(t), C_B(t), C_C(t)) \\
\frac{dC_B(t)}{dt} &= H(C_A(t), C_B(t), C_C(t), A_m(t))
\end{aligned}
$$

Linearizing the system around the steady state C_A^{SS}, C_B^{SS}, C_C^{SS} and A_m^{SS} and introducing

$$
\begin{aligned}
\delta C_i &= C_i - C_i^{SS} \\
\delta A_m &= A_m - A_m^{SS}
\end{aligned}
$$

The linearized system around the deviation then looks like

$$
\begin{aligned}
\frac{d\delta C_A(t)}{dt} &= \left.\frac{\partial F(C_A(t), C_B(t), C_C(t))}{\partial C_A}\right|_{C_A^{SS}, C_B^{SS}, C_C^{SS}, A_m^{SS}} (C_A - C_A^{SS}) \\
&+ \left.\frac{\partial F(C_A(t), C_B(t), C_C(t))}{\partial C_B}\right|_{C_A^{SS}, C_B^{SS}, C_C^{SS}, A_m^{SS}} (C_B - C_B^{SS}) \\
&+ \left.\frac{\partial F(C_A(t), C_B(t), C_C(t))}{\partial C_C}\right|_{C_A^{SS}, C_B^{SS}, C_C^{SS}, A_m^{SS}} (C_C - C_C^{SS}) \\
\frac{d\delta C_B(t)}{dt} &= \left.\frac{\partial H(C_A(t), C_B(t), C_C(t))}{\partial C_A}\right|_{C_A^{SS}, C_B^{SS}, C_C^{SS}, A_m^{SS}} (C_A - C_A^{SS}) \\
&+ \left.\frac{\partial H(C_A(t), C_B(t), C_C(t))}{\partial C_B}\right|_{C_A^{SS}, C_B^{SS}, C_C^{SS}, A_m^{SS}} (C_B - C_B^{SS}) \\
&+ \left.\frac{\partial H(C_A(t), C_B(t), C_C(t))}{\partial C_C}\right|_{C_A^{SS}, C_B^{SS}, C_C^{SS}, A_m^{SS}} (C_C - C_C^{SS}) \\
&+ \left.\frac{\partial H(C_A(t), C_B(t), C_C(t))}{\partial A_m}\right|_{C_A^{SS}, C_B^{SS}, C_C^{SS}, A_m^{SS}} (A_m - A_m^{SS})
\end{aligned}
$$

By computing these partial derivatives, you become

$$
\begin{aligned}
\frac{d\delta C_A(t)}{dt} &= \frac{1}{V}(-q\delta C_A - 4k_1 C_A^{SS}\delta C_A + 2k_2 C_C^{SS}\delta C_B + 2k_2 C_B^{SS}\delta C_C), \\
\frac{d\delta C_B(t)}{dt} &= \frac{1}{V}(-q\delta C_B + 2k_1 C_A^{SS}\delta C_A - k_2 C_C^{SS}\delta C_B - k_2 C_B^{SS}\delta C_C) - K_m A_m^{SS}\delta C_B - K_m C_B^{SS}\delta A_m.
\end{aligned}
$$