Stability Analysis via Linearization Examples

(tbco 2/16/2021)

Motivation: Several process models used in chemical engineering are nonlinear and multivariable. Further, some important cases include those where there are multiple steady states that are possible. Unfortunately, some of the steady states might be an unstable point, thus requiring a control system to both stabilize and control the process at and around that chosen operating point. One method to predict the stability of operating points is to use linearized models and apply multivariable analysis to assess the local behavior around these operating points.

Example 1:

A bioreactor was modeled with the following set of differential equation

$$\frac{dC}{dt} = \left(\left[\frac{\mu_{max}S}{k_m + S + k_1 S^2} \right] - D \right) C$$

$$\frac{dS}{dt} = D(S_{in} - S) - \left[\frac{\mu_{max}S}{k_m + S + k_1 S^2} \right] \frac{C}{Y}$$
(1)

where C is the cell-concentration (g/liter) and S is the substrate-concentration (g/liter). Both C and S are the process variables, while the other terms are fixed parameters given by

$0.53 hr^{-1}$
0.12 g/liter
0.454 liter/g
0.4
$0.3 hr^{-1}$
4 g/liter

(Note: the dilution rate is a potential candidate to be the controller output while S_{in} is a potential candidate to be the disturbance. However, with both treated as parameters, we are essentially performing an open-loop analysis.)

A) Steady-state analysis

By setting the time-derivatives to zero, we need to satisfy the following equations simultaneously:

$$\left(\left[\frac{\mu_{max}S_{ss}}{k_m + S_{ss} + k_1S_{ss}^2}\right] - D\right)C_{ss} = 0$$

$$D(S_{in} - S_{ss}) - \left[\frac{\mu_{max}S_{ss}}{k_m + S_{ss} + k_1S_{ss}^2}\right]\frac{C_{ss}}{Y} = 0$$
(2)

From the first nonlinear equation, we have two cases: either $C_{ss} = 0$ or $C_{ss} \neq 0$.

For $C_{ss} = 0$, then the second equation immediately yields $S_{ss} = S_{in}$. Thus, one steady state is at $(C_{ss}, S_{ss}) = (0, S_{in})$.

For $C_{ss} \neq 0$, we need (assuming $D \neq 0$)

$$\left[\frac{\mu_{max}S_{ss}}{k_m + S_{ss} + k_1S_{ss}^2}\right] - D = 0 \quad \to \quad k_1S_{ss}^2 + \left(1 - \frac{\mu_{max}}{D}\right)S_{ss} + k_m = 0$$

which will yield two roots, say S_{ss_2} and S_{ss_3} .

The corresponding values of C_{ss} will result from the second equation in (2),

$$C_{ss_2} = (S_{in} - S_{ss_2})Y$$
 and $C_{ss_3} = (S_{in} - S_{ss_3})Y$

Using the given values, we thus have 3 steady states given by:

Steady state 1: $(C_{ss}, S_{ss}) = (0, 4)$

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Steady state 2: (C_{ss}, S_{ss}) = (0.994, 1.514)
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Steady state 3: $(C_{ss}, S_{ss}) = (1.53, 0.175)$

Remarks:

- 1) Steady state 1 indicates that no cells are present a cell-extinction scenario.
- 2) Steady state 2 indicates medium cell growth and medium reduction in substrate concentration compared to the feed.
- Steady state 3 indicates high cell growth together with significant reduction of substrate.

B) Linearized models based on operating at the steady states

We can obtain three different approximate linear models by linearizing the original model at the three steady states.

Following the procedures discussed in lecture 8, we have

Operating around steady state 1:

$$\frac{dC}{dt} = -(0.1138)C$$
$$\frac{dS}{dt} = -(0.4656)C - (0.3)S + 1.2$$

Operating around steady state 2:

$$\frac{dC}{dt} = (8.563 \times 10^{-6})C - (0.06779)S + 0.1026$$
$$\frac{dS}{dt} = -(0.750)C - (0.1305)S + 0.9434$$

Operating around steady state 3:

$$\frac{dC}{dt} = (2.553 \times 10^{-4})C + (0.9016)S - 0.1578$$
$$\frac{dS}{dt} = -(0.7506)C - (2.5540)S + 1.5944$$

C) Local Stability Analysis around Steady States

We can generalize the three linearized equations to have the following indexed coefficient form:

$$\frac{dC}{dt} = a_{11}C + a_{12}S + b_1$$
$$\frac{dS}{dt} = a_{21}C + a_{22}S + b_2$$

and can show using the method in lecture 8 to yield the following characteristic equation:

$$\lambda^2 - (a_{11} + a_{22})\lambda + (a_{11}a_{22} - a_{12}a_{21}) = 0$$

Thus, we have the following characteristic equations and eigenvalues associated with the three different steady states:

Steady state 1:

	$\lambda^{2} + 0.4138\lambda + 0.0341 = 0$ $\rightarrow \lambda = -0.3, -0.114$
Steady state 2:	$\lambda^{2} + 0.1305\lambda - 0.0508 = 0$ $\rightarrow \lambda = 0.1695, -0.3$
Steady state 3:	$\lambda^2 + 2.554\lambda + 0.6760 = 0$ $\rightarrow \lambda = -2.2538, -0.2999$

D) Summary of example 1

Steady state 1: $(C_{ss}, S_{ss}) = (0, 4), \ \lambda = -0.3, -0.114$ Steady state 2: $(C_{ss}, S_{ss}) = (0.994, 1.514), \ \lambda = 0.1695, -0.3$ Steady state 3: $(C_{ss}, S_{ss}) = (1.53, 0.175), \ \lambda = -2.2538, -0.2999$

Remarks:

- 1) Steady state 2 is unstable. Any initial conditions starting around this operating point will either get attracted towards steady state 1 or steady state 3.
- 2) Steady state 1 is undesirable since it means a depletion of cells towards extinction even if it initially had starter population.
- If steady state 3 is the desirable operating situation, initial charging of the bioreactor has to be between steady state 2 and steady state 3 so that extinction is avoided.
- 4) If for some reason (for academic purposes perhaps) one desires to operate at the steady state 2, a feedback control should be set-up to stabilize the process by manipulating, for instance, the dilution rate to keep cell and substrate concentrations close to steady state 2. Once stabilized, a cascaded PID control set-up could be included to control the system to setpoints around this operating point.

Example 2:

A CSTR undergoes a non-isothermal second order reaction from a compound A to form product B is modeled with the following set of differential equation

$$\frac{dC}{dt} = {\binom{F}{V}}(C_{in} - C) - k_o \exp\left(-\frac{E}{R(T + 273)}\right)C^2$$

$$\frac{dT}{dt} = {\binom{F}{V}}(T_{in} - T) - \frac{k_o \exp\left(-\frac{E}{R(T + 273)}\right)C^2 \Delta H_{rxn}}{\rho C_p V} + \frac{UA}{\rho C_p V}(T_J - T)$$
(3)

where C is the cell-concentration (g/liter) and S is the substrate-concentration (g/liter). Both C and S are the process variables, while the other terms are fixed parameters given by

F/V	50 <i>s</i>
E/R	2600 K
k _o	$1750 \ liter/(g \cdot s)$
$\beta = \Delta H_{rxn} / (\rho C_p V)$	$-1530 \ liter \cdot ^{\circ}C/g$
$\gamma = UA/(\rho C_p V)$	$3 s^{-1}$
T _{in}	25 ° <i>C</i>
C _{in}	1 g/liter
	25° <i>C</i>

(Note: the heat rate q is a potential candidate to be the controller output while T_{in} and C_{in} are potential candidates to be the disturbance. However, with both treated as parameters, we are essentially performing an open-loop analysis.)

A) <u>Steady-state analysis</u>

By setting the time-derivatives to zero, we need to satisfy the following equations simultaneously:

$$\begin{pmatrix} \overline{F}\\ \overline{V} \end{pmatrix} (C_{in} - C_{ss}) - k_o \exp\left(-\frac{E}{R(T_{ss} + 273)}\right) C_{ss}^2 = 0$$

$$\begin{pmatrix} \overline{F}\\ \overline{V} \end{pmatrix} (T_{in} - T_{ss}) - \frac{k_o \exp\left(-\frac{E}{R(T_{ss} + 273)}\right) C_{ss}^2 \Delta H_{rxn}}{\rho C_p V} + \frac{UA}{\rho C_p} (T_J - T_{ss}) = 0$$

$$(4)$$

Let $\sigma = k_o \exp(-E/(R(T + 273)))$ be the Arhenius rate constant, then from the first nonlinear equation, we can obtain the positive solutions for C_{ss} ,

$$C_{ss}(T_{ss}) = h_1(T_{ss}) = \frac{\left(-\left(\frac{F}{V}\right) + \sqrt{\left(\frac{F}{V}\right)^2 + 4\sigma(T_{ss})\left(\frac{F}{V}\right)C_{in}}\right)}{2\sigma(T_{ss})}$$
(5)

Next, from (4), solving for σ from the first equation and then substituting it to the second equation, we get

$$C_{ss}(T_{ss}) = h_2(T_{ss})$$

$$= \left(\frac{UA}{\Delta H_{rxn}} \left(\frac{V}{F}\right) + \frac{\rho C_p V}{\Delta H_{rxn}}\right) T_{ss} + \left(C_{in} - \frac{UA}{\Delta H_{rxn}} \left(\frac{V}{F}\right) T_J - \frac{\rho C_p V}{\Delta H_{rxn}} T_{in}\right)$$
(6)

By plotting h_1 and h_2 in the same graph as shown in Figure 1, the intersections will be the steady states. Using initial guesses close to the intersection points, a nonlinear solver should be able to yield the steady states.



Figure 1. Plot of $h_1(T)$ and $h_2(T)$ to reveal steady states at the intersection points.

The 3 steady states are then found to be:

Steady state 1: $(C_{ss}, T_{ss}) = (0.992 \ g/liter, 36.0^{\circ}C)$ Steady state 2: $(C_{ss}, T_{ss}) = (0.864 \ g/liter, 221.8^{\circ}C)$ Steady state 3: $(C_{ss}, T_{ss}) = (0.4 \ g/liter, 891^{\circ}C)$

Remarks:

- 1) Steady state 1 has a very low conversion (almost none).
- 2) Steady state 2 has a low conversion as well, around 14%.
- 3) Steady state 3 has the highest conversion of around 60%. However, this occurs at $T = 891^{\circ}C$, a very high and potentially dangerous temperature.

B) Linearized models based on operating at the steady states

We can obtain three different approximate linear models by linearizing the original model at the three steady states.

Following the procedures discussed in lecture 8, we have

Operating around steady state 1:

$$\frac{dC}{dt} = -50.77C - 0.010T + 50.76$$
$$\frac{dT}{dt} = 1179.2C - 37.07T + 165.98$$

Operating around steady state 2:

$$\frac{dC}{dt} = -(65.76)C - (0.07238)T + 72.85$$
$$\frac{dT}{dt} = (2.411 \times 10^4)C + 57.74T - 3.363 \times 10^4$$

Operating around steady state 3:

$$\frac{dC}{dt} = -(199.6)C - (0.05761)T + 131.2$$
$$\frac{dT}{dt} = (2.290 \times 10^5)C + (35.15)T - 1.230 \times 10^5$$

C) Local Stability Analysis around Steady States

We can generalize the three linearized equations to have the following indexed coefficient form:

$$\frac{dC}{dt} = a_{11}C + a_{12}S + b_1$$
$$\frac{dT}{dt} = a_{21}C + a_{22}T + b_2$$

and can show using the method in lecture 8 to yield the following characteristic equation:

$$\lambda^2 - (a_{11} + a_{22})\lambda + (a_{11}a_{22} - a_{12}a_{21}) = 0$$

Thus, we have the following characteristic equations and eigenvalues associated with the three different steady states:

Steady state 1:

	$\lambda^{2} + 87.84\lambda + 1894 = 0$ $\rightarrow \lambda = -49.84, -37.99$
Steady state 2:	$\lambda^2 + 8.02\lambda - 2052 = 0$ $\rightarrow \lambda = -49.49, 41.47$
Steady state 3:	$\lambda^2 + 164.4\lambda + 6177 = 0$ $\rightarrow \lambda = -106.4, -58.05$

D) Summary of example 2

Steady state 1: $(C_{ss}, T_{ss}) = (0.992 \ g/liter, 36.0^{\circ}C), \lambda = -49.84, -37.99$ Steady state 2: $(C_{ss}, T_{ss}) = (0.864 \ g/liter, 221.8^{\circ}C), \lambda = -49.49, 41.47$ Steady state 3: $(C_{ss}, T_{ss}) = (0.4 \ g/liter, 891^{\circ}C), \lambda = -106.4, -58.05$

Remarks:

- 1) Steady state 2 is unstable. Any initial conditions starting around this operating point will either get attracted towards steady state 1 or steady state 3.
- 2) Steady state 1 is not desirable since it has a very low conversion.
- 3) Steady state 3 is not desirable either because the temperature is getting dangerously hot.
- 4) Steady state 2 might need to be explored further. Recycling of unreacted material may be needed to increase overall conversion. However, since it is unstable, a feedback control is needed to stabilize the process.
- 5) This occurs only for exothermic reactions, although some exothermic reactions can still operate with a higher conversion but not too high of a temperature condition.
- 6) The main point is this: if one relies only on steady-state calculations and arbitrarily decided on any of these points without testing for stability, the design may end up missing important and significant safety and control costs.