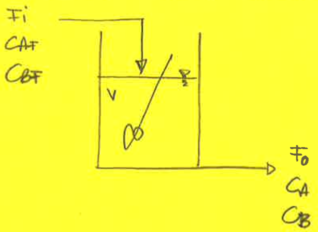
CSTR FIRST-ORDER IRREVERSIBLE REACTION



Consider a single irreversible reaction $A \to B$

→ Assume a rate of generation per unit volume that is first order with respect to C_A

⇝ MOLAR RATE OF REACTION OF A PER UNIT VOLUME $= r_A$

$$r_A = K C_A$$

→ EACH MOLE OF A CREATES A MOLE OF B

⇝ MOLAR RATE OF FORMATION OF B PER UNIT VOLUME $= r_B$

$$r_B = K C_A$$

WE START BY WRITING THE DYNAMIC MODELLING EQUATIONS

$\boxed{\text{COMPONENT A}}$

$$\frac{dVC_A}{dt} = FC_{AF} - FC_A - VkC_A$$

(WITH k THE REACTION RATE CONSTANT)

ASSUMING THAT V IS CONSTANT, WE HAVE $(F_i = F_o)$

$$\frac{dC_A}{dt} = \frac{F}{V}C_{AF} - \frac{F}{V}C_A - KC_A = \frac{F}{V}C_{AF} - \left(\frac{F}{V} + k\right)C_A$$

$\boxed{\text{COMPONENT B}}$

$$\frac{dVC_B}{dt} = FC_{BF} - FC_B + VKC_A$$

ASSUMING CONSTANT VOLUME AND NO B IN THE ~~FEED~~ →

$$\frac{dC_B}{dt} = -\frac{F}{V}C_B + KC_A$$

1

$$\begin{cases} \dfrac{dC_A}{dt} = \dfrac{F}{V}C_{AF} - \left(\dfrac{F}{V} + k\right)C_A \\ \dfrac{dC_B}{dt} = -\dfrac{F}{V}C_B + KC_A \end{cases}$$

The concentration of B does not play any role in the dynamics of component A

$$\begin{bmatrix} \dot{C}_A \\ \dot{C}_B \end{bmatrix} = \begin{bmatrix} F/V\, C_{AF} - (F/V + K)C_A \\ -F/V\, C_B + KC_A \end{bmatrix}$$

OR $\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} C_A \\ C_B \end{bmatrix}, \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} F \\ C_{AF} \end{bmatrix}$

$\theta = [K, V]$

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} u_1/V\, u_2 - (u_1/V + k)x_1 \\ -u_1/V\, x_2 + kx_1 \end{bmatrix} = \begin{bmatrix} f_1(x_1, x_2, u_1, u_2 \mid \theta_1, \theta_2) \\ f_2(x_1, x_2, u_1, u_2 \mid \theta_1, \theta_2) \end{bmatrix}$$

BASIC LINEARIZATION AROUND A FIXED POINT

$$A = \begin{bmatrix} \left.\dfrac{\partial f_1}{\partial x_1}\right|_{ss} & \left.\dfrac{\partial f_1}{\partial x_2}\right|_{ss} \\ \left.\dfrac{\partial f_2}{\partial x_1}\right|_{ss} & \left.\dfrac{\partial f_2}{\partial x_2}\right|_{ss} \end{bmatrix} \qquad B = \begin{bmatrix} \partial f_1/\partial u_1|_{ss} & \partial f_1/\partial u_2|_{ss} \\ \partial f_2/\partial u_1|_{ss} & \partial f_2/\partial u_2|_{ss} \end{bmatrix}$$

$\partial f_1/\partial x_1 = -u_1/V - K$
$\partial f_1/\partial x_2 = 0$
$\partial f_2/\partial x_1 = k$
$\partial f_2/\partial x_2 = -u_1/V$

$\partial f_1/\partial u_1 = u_2/V - x_1/V$
$\partial f_1/\partial u_2 = u_1/V$
$\partial f_2/\partial u_1 = -x_2/V$
$\partial f_2/\partial u_2 = 0$

$u_1/V|_{ss} = 0.2\ \text{min}^{-1}$

$u_2|_{ss} = 1.0\ \dfrac{\text{gmol}}{\text{lt}}$

$k = 0.2\ \text{min}^{-1}$

$$A = \begin{bmatrix} -0.4 & 0 \\ 0.2 & -0.2 \end{bmatrix}$$

$$B = \begin{bmatrix} ** & 0.2 \\ ** & 0 \end{bmatrix}$$

TO BE COMPUTED → SEE 2

WE ASSUME THAT F/V IS THE CONTROL VARIABLE OF INTEREST

- F/V IS CALLED SPACE VELOCITY
- V/F IS CALLED RESIDENCE TIME

$\rightarrow$ CONSIDER $\frac{dC_A}{dt} = \frac{F}{V} C_{AF} - \left(\frac{F}{V} + k\right) C_A$ AND ASSUME STEADY-STATE CONDITIONS

- THAT IS $dC_A/dt = 0$, WE HAVE $C_A^{ss} = \frac{F/V^{ss} C_{AF}^{ss}}{F/V^{ss} + K}$

- AS F^{ss}/V GETS LARGER (MORE FEED), C_A^{ss} TENDS TO C_{AF}^{ss}
(the flow is so fast, that there is no conversion)

- AS F^{ss}/V GETS SMALLER (LESS FEED), C_A^{ss} TENDS TO ZERO
(the flow is so slow, that everything gets converted)

N.B $F^{ss}/V = 0$ MEANS $F^{ss} = 0$ $\rightsquigarrow$ BATCH REACTOR

The steady-state gain (INPUT-OUTPUT) is the derivative of C_A^{ss} wrt F^{ss}/V

$$* \quad \frac{\partial C_A^{ss}}{\partial F^{ss}/V} = \frac{K C_{AF}^{ss}}{(KV/F^{ss} + K)^2}$$

The steady-state gain (DISTURBANCE-OUTPUT) is the derivative of C_A^{ss} wrt C_{AF}^{ss}

$$* \quad \frac{\partial C_A^{ss}}{\partial C_{AF}^{ss}} = \frac{KV/F^{ss}}{KV/F^{ss} + K}$$

$K = 0.2 \text{ min}^{-1}$
$F^{ss}/V = 0.2 \text{ min}^{-1}$

$$* \quad b_{11} = \left.\frac{\partial f_1}{\partial u_1}\right|_{ss} = \left. u_2/V - x_1/V \right|_{ss} = \frac{1}{V}\left(u_2^{ss} - x_1^{ss}\right)$$

$u_2^{ss} = C_{AF}^{ss} = 1.0$

$$x_1^{ss} = C_A^{ss} = \frac{F^{ss}/V \cdot (C_{AF}^{ss})}{F^{ss}/V + K} = \frac{(0.2)\cdot(1.0)}{0.2 + 0.2} = \frac{0.2}{0.4} = 0.50$$

$$\rightsquigarrow \boxed{b_{11} = \frac{1}{V} \cdot \frac{1}{6}}$$

$$\boxed{* \quad b_{21} = -u_2/V = -\frac{1}{V} u_2^{ss} = -\frac{1}{V}}$$

→ CONSIDER $\frac{dC_B}{dt} = -\frac{F}{V} C_B + K C_A$ AND ASSUME STEADY STATE COND.

– THAT IS $dC_B/dt = 0$, WE HAVE $C_B^{ss} = \frac{K C_A^{ss}}{F^{ss}/V}$ WITH C_A^{ss}

$$C_A^{ss} = \frac{F^{ss}/V \; C_{AF}^{ss}}{F^{ss}/V + K}$$, BY SUBSTITUTION WE HAVE $X_1^{ss} = \frac{0.2 \cdot 1}{0.2 + 0.2} = \frac{0.2}{0.4} = 0.5$

$$C_B^{ss} = \frac{K}{F^{ss}/V} \frac{F^{ss}/V \,(C_{AF}^{ss})}{F^{ss}/V + K} = \frac{K C_{AF}^{ss}}{F_s/V + K}$$ $\longrightarrow X_2^{ss} = \frac{0.2 * 1}{0.2 + 0.2} = 0.5$

– AS F^{ss}/V GETS LARGER, C_B^{ss} TENDS TO ZERO

– AS F^{ss}/V GETS SMALLER, C_B^{ss} APPROACHES C_{AF}^{ss}

LINEARISATION AROUND A STEADY-STATE (FIXED POINT)

Define $\begin{cases} x_1 = C_A - C_A^{ss} \\ x_2 = C_B - C_B^{ss} \end{cases}$, we have $\begin{cases} \dot{x}_1 = dC_A/dt - 0 \\ \dot{x}_2 = dC_B/dt - 0 \end{cases}$

Also define $\begin{cases} u_1 = F - F^{ss} \\ u_2 = C_{AF} - C_{AF}^{ss} \end{cases}$

WE HAVE, BY SUBSTITUTING AND LINEARISING:

$$\frac{dx_1}{dt} = -\left(\frac{F^{ss}}{V} + K\right) x_1 + (C_{AF} - C_A^{ss}) u_1 + \frac{F^{ss}}{V} u_2$$

$$\frac{dx_2}{dt} = K x_1 + \left(-\frac{F^{ss}}{V}\right) x_2 - C_B^{ss} u_1$$

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} -(F^{ss}/V + K) & 0 \\ K & -F^{ss}/V \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} C_{AF}^{ss} - C_A^{ss} & F^{ss}/V \\ -C_B^{ss} & 0 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

$$= \begin{bmatrix} -0.4 & 0 \\ 0.2 & -0.2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} 0.5 & 0.2 \\ -0.5 & 0 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

$$\frac{dC_A}{dt} = \frac{F}{V} C_{AF} - \left(\frac{F}{V} + K\right) C_A$$

$$\frac{dC_B}{dt} = -\frac{F}{V} C_B + k C_A$$

let $x_1 = C_A$
$x_2 = C_B$

let $u_1 = F/V$
$u_2 = C_{AF}$

$u_1^{ss} = 0.2 \text{ min}^{-1}$
$u_2^{ss} = 1 \text{ gmol/lt}$
$K = 0.2 \text{ min}^{-1}$

$$\frac{dx_1}{dt} = \underbrace{u_1 u_2 - (u_1 + k) x_1}_{f_1(x_1, x_2, u_1, u_2)}$$

$$\frac{dx_2}{dt} = \underbrace{-u_1 x_2 + k x_1}_{f_2(x_1, x_2, u_1, u_2)}$$

$$\frac{dx_1}{dt} \approx f_1(x^{ss}, u^{ss}) + \left.\frac{\partial f_1}{\partial x_1}\right|_{ss} (x_1 - x_1^{ss}) + \left.\frac{\partial f_1}{\partial x_2}\right|_{ss} (x_2 - x_2^{ss}) + \left.\frac{\partial f_1}{\partial u_1}\right|_{ss} (u_1 - u_1^{ss}) + \left.\frac{\partial f_1}{\partial u_2}\right|_{ss} (u_2 - u_2^{ss}) + \cdots$$

$$\frac{dx_2}{dt} \approx f_2(x^{ss}, u^{ss}) + \left.\frac{\partial f_2}{\partial x_1}\right|_{ss} (x_1 - x_1^{ss}) + \left.\frac{\partial f_2}{\partial x_2}\right|_{ss} (x_2 - x_2^{ss}) + \left.\frac{\partial f_2}{\partial u_1}\right|_{ss} (u_1 - u_1^{ss}) + \left.\frac{\partial f_2}{\partial u_2}\right|_{ss} (u_2 - u_2^{ss}) + \cdots$$

$$\frac{\partial f}{\partial x} = \begin{bmatrix} -(u_1 + K) & 0 \\ K & -u_1 \end{bmatrix} \xrightarrow{ss} \begin{bmatrix} -(0.2 + 0.2) \; [-0.4] & 0 \\ 0.2 & -0.2 \end{bmatrix}$$

$$\frac{\partial f}{\partial u} = \begin{bmatrix} u_2 - x_1 & u_1 \\ -x_2 & 0 \end{bmatrix} \xrightarrow{ss} \begin{bmatrix} 1 - 0.5 \; [0.5] & 0.2 \\ 0.5 & 0 \end{bmatrix}$$

let $\begin{cases} x_1' = x_1 - x_{1ss} \\ x_2' = x_2 - x_{2ss} \end{cases}$ let $\begin{cases} u_1' = u_1 - u_1^{ss} \\ u_2' = u_2 - u_2^{ss} \end{cases}$

$$\frac{dx_1'}{dt} = \frac{dx_1}{dt}$$

$$\frac{dx_2'}{dt} = \frac{dx_2}{dt}$$

$$\frac{dx_1'}{dt} \approx \left.\frac{\partial f_1}{\partial x_1}\right|_{ss} x_1' + \left.\frac{\partial f_1}{\partial x_2}\right|_{ss} x_2' + \left.\frac{\partial f_1}{\partial u_1}\right|_{ss} u_1' + \left.\frac{\partial f_1}{\partial u_2}\right|_{ss} u_2'$$

$$\frac{dx_2'}{dt} = \left.\frac{\partial f_2}{\partial x_1}\right|_{ss} x_1' + \left.\frac{\partial f_2}{\partial x_2}\right|_{ss} x_2' + \left.\frac{\partial f_2}{\partial u_1}\right|_{ss} u_1' + \left.\frac{\partial f_2}{\partial u_2}\right| u_2'$$

$$\begin{bmatrix} x_1' \\ x_2' \end{bmatrix} = \underbrace{\begin{bmatrix} -0.4 & 0 \\ 0.2 & -0.2 \end{bmatrix}}_{A} \begin{bmatrix} x_1' \\ x_2' \end{bmatrix} + \underbrace{\begin{bmatrix} 0.5 & 0.2 \\ 0.5 & 0 \end{bmatrix}}_{B} \begin{bmatrix} u_1' \\ u_2' \end{bmatrix}$$

$$x'(t) = \underbrace{e^{At} x'(0)}_{FF} + \int_0^t e^{A(t-\tau)} B\, u(\tau)\, d\tau$$

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>> syms t
>> A = [-0.4 0; 0.2 -0.2];
>> expmAt = expm(A*t)
>> x0 = [1; 1]
>> x_u = expmAt * x0
>> fplot(x_u, [0,10])
```

FORCE - FREE RESPONSE

DISCOVER IN CLASS HOW TO DO THE FORCED RESPONSE