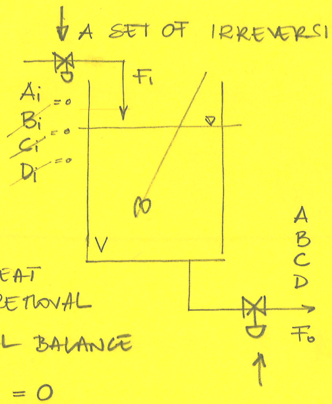
ISOTHERMAL CSTR

$$\begin{cases} A \xrightarrow{k_1} B \xrightarrow{k_2} C \\ 2A \xrightarrow{k_3} D \end{cases}$$

↓ A SET OF IRREVERSIBLE REACTIONS



— CONSTANT DENSITY

— CONSTANT VOLUME

B is THE PRODUCT

SIMPLIFIED — NO HEAT REMOVAL

TOTAL MATERIAL BALANCE

$$\frac{dV}{dt} = F_i - F_o = 0$$

COMPONENT A BALANCE

$$\frac{dVC_A}{dt} = FC_{Ai} - FC_A \underbrace{- Vk_1C_A - Vk_3C_A^2}_{r_A}$$

mol/(min lt)

$$\rightarrow \frac{dC_A}{dt} = \frac{F}{V}[C_{Ai} - C_A] - k_1C_A - k_3C_A^2$$

COMPONENT B BALANCE

$$\rightarrow \frac{dC_B}{dt} = \frac{F}{V}[\cancel{C_{Bi}} - C_B] \underbrace{+ k_1C_A - k_2C_B}_{r_B}$$

COMPONENT C BALANCE

$$\rightarrow \frac{dC_C}{dt} = \frac{F}{V}[\cancel{C_{Ci}} - C_C] \underbrace{+ k_2C_B}_{r_C}$$

COMPONENT D BALANCE

$$\rightarrow \frac{dC_D}{dt} = \frac{F}{V}[\cancel{C_{Di}} - C_D] \underbrace{+ \frac{1}{2}k_3C_A^2}_{r_D}$$

$k_1 = 5/6$ min^{-1}

$k_2 = 5/3$ min^{-1}

$k_3 = 1/6$ $lt(mol^{-1}\,min^{-1})$

RATE CONSTANTS

$$\frac{mol}{lt}\,\frac{mol}{lt}\left(\frac{lt}{mol}\right) \equiv \frac{mol}{lt\ min}$$

$r_{A,B,C,D}$

rate of 'generation' of A, B, C, D per unit volume

$k_1 = 5/6$

$k_2 = 5/3$

$k_3 = 1/6$

$F^{ss}/V = 4/7$ min^{-1}

$\boxed{C_{Af}^{ss} = 10}$ mol/lt

$C_{Ass} = 3$ mol/l

$C_{Bss} = 1.1140$ mol/l

$C_{Css} = 3.2580$ mol/lt

$C_{Dss} = 1.3125$ mol/lt

$$dC_A/dt = F/V\,(C_{Ai} - C_A) - K_1 C_A - K_3 C_A^2$$

$$dC_B/dt = F/V\,(-C_B) + K_1 C_A - K_2 C_B$$

$$dC_C/dt = F/V\,(-C_C) + K_2 C_B$$

$$dC_D/dt = F/V\,(-C_D) + 1/2\,K_3 C_A^2$$

STATES

C_A, C_B, C_D, C_C

INPUTS

F or F/V

PARAMETERS

K_1, K_2, K_3

Assume that B is desired product and thus we measure its concentration (only)

$$\boxed{y = C_B}$$

STEADY STATE CONDITIONS

* $\frac{dC_A}{dt} = 0 \rightsquigarrow \frac{F}{V}\left[C_{Ai} - C_A\right] - K_1 C_A - K_3 C_A^2 = 0$

$$-K_3 C_A^2 - C_A\left[\frac{F}{V} + K_1\right] + \frac{F}{V} C_{Ai} = 0$$

$$\underbrace{K_3}_{a} C_A^2 + \underbrace{\left[\frac{F}{V} + K_1\right]}_{b} C_A \underbrace{- \frac{F}{V} C_{Ai}}_{c} = 0$$

$$ax^2 + bx + c = 0$$

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

CONSIDER THE POSITIVE ROOT

$$\boxed{C_A^{SS}} = \frac{-\left(K_1 + \frac{F^{SS}}{V}\right)}{2K_3} + \frac{\sqrt{(K_1 + F^{SS}/V)^2 + 4K_3 (F^{SS}/V)\, C_{Ai}^{SS}}}{2K_3}$$

* $dC_B/dt \rightsquigarrow -C_B\left[\frac{F}{V} + K_2\right] + K_1 C_A = 0$

$$\left[F^{SS}/V + K_2\right] C_B^{SS} - K_1 C_A^{SS} = 0$$

$$\boxed{C_B^{SS}} = K_1 C_A^{SS} \Big/ \left[F^{SS}/V + K_2\right]$$

$$= \frac{K_1\left[\frac{-K_1 + F^{SS}/V}{2K_3} + \frac{\sqrt{(K_1 + F^{SS}/V)^2 + 4K_3 (F^{SS}/V)\, C_{Ai}^{SS}}}{2K_3}\right]}{\left[F^{SS}/V + K_2\right]}$$

* $dC_C/dt = 0 \rightsquigarrow -C_C\left[F/V\right] + K_2 C_B = 0$

$$F/V\, C_C - K_2 C_B = 0$$

$$\boxed{C_C^{ss}} = K_2 C_B^{ss} / (F^{ss}/V)$$

$$= \frac{K_2 \left[\frac{-K_1 + F^{ss}/V}{2K_3} + \frac{\sqrt{(K_1+F^{ss}/V)^2 + 4K_3(F^{ss}/V)\, C_{A_i}^{ss}}}{2K_3} \right] / \left[\frac{F^{ss}/V}{K_2} + \right]}{F^{ss}/V}$$

* $dC_D/dt = 0 \rightsquigarrow -\frac{F}{V} C_D + \frac{1}{2} K_3 C_A^2 = 0$

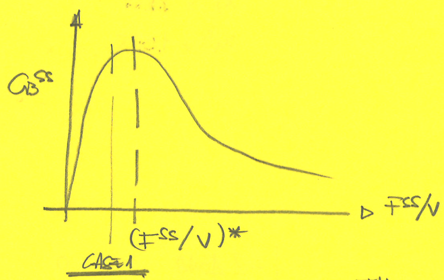
$$F/V\, C_D - 1/2\, K_3 C_A^2 = 0$$

$$\boxed{C_D^{ss}} = \frac{1/2\, K_3\, C_A^{ss\,2}}{(F^{ss}/V)}$$

$$= \frac{1/2\, K_3 \left[\quad / \quad \right]^2}{F^{ss}/V}$$

PLOT THE STEADY STATE CONCENTRATION OF C_B (C_B^{ss}) AS A FUNCTION OF THE STATE VELOCITY (F^{ss}/V)

BY STUDYING THE EXPRESSION OF C_B^{ss} (and C_A^{ss}, C_C^{ss} and C_D^{ss}) AS FUNCTION OF F^{ss}/V WE CAN DERIVE THE SO-CALLED INPUT-OUTPUT CURVE



IT IS EASY TO SEE THAT THERE IS A MAXIMUM VALUE OF THE CONCENTRATION OF B

$\longrightarrow$ IF THE OBJECTIVE IS TO MAXIMIZE THE PRODUCTION OF B, THEN THERE EXISTS AN OPTIMUM RESIDENCE TIME (~ 1.292 min^{-1})

THE LINEAR STATE SPACE MODEL OF THE NONLINEAR REPRESENTATION

$$\dot{x} = Ax + Bu$$
$$y = Cx$$

WE FIRST DEFINE THE VARIABLES

$$x = \begin{bmatrix} C_A - C_A^{ss} \\ C_B - C_B^{ss} \end{bmatrix} \quad \left(\begin{bmatrix} C_A - C_A^{ss} \\ C_B - C_B^{ss} \\ C_C - C_C^{ss} \\ C_D - C_D^{ss} \end{bmatrix} \right)$$

$$u = \left[F/V - F^{ss}/V \right]$$

$$y = \begin{bmatrix} C_A - C_A^{ss} \\ C_B - C_B^{ss} \end{bmatrix}$$

$$dC_A/dt = F/V\,(C_{Ai} - C_A) - k_1 C_A - K_3 C_A^2$$
$$dC_B/dt = F/V\,(-C_B) + k_1 C_A - K_2 C_B$$
$$dC_C/dt = F/V\,(-C_C) + K_2 C_B$$
$$dC_D/dt = F/V\,(-C_B) + 1/2\, K_3 C_A^2$$

THE DYNAMICS

$x_1^{ss} = 3$ $\qquad u_1^{ss} = 4/7$

$x_2^{ss} = 1.117$ $\qquad u_2^{ss} = 10$

$x_3^{ss} = 3.258$

$x_4^{ss} = 1.3125$

$$A = \begin{bmatrix} -2.4048 & 0 & 0 & 0 \\ 5/6 & -2.2381 & 0 & 0 \\ 0 & 5/3 & -4/4 & 0 \\ 0.5 & 0 & 0 & -4/7 \end{bmatrix}$$

$$B = \begin{bmatrix} 7 & 10 \\ -1.117 & 0 \\ -3.258 & 0 \\ -1.3125 & 0 \end{bmatrix}$$

$$\frac{d\overset{x_1}{C_A}}{dt} = u_1(\overset{u_2}{C_{A1}} - x_1) - k_1 x_1 - k_3 x_1^2$$

$$\frac{d\overset{x_2}{C_B}}{dt} = u_1(-x_2) + k_1 x_1 - k_2 x_2$$

$$\frac{d\overset{x_3}{C_C}}{dt} = u_1(-x_3) + k_2 x_2$$

$$\frac{d\overset{x_4}{C_D}}{dt} = u_1(-x_4) + \frac{1}{2} k_3 x_1^2$$

$$\frac{\partial f_1}{\partial x_1} = -u_1^{ss} - k_1 - 2k_3 x_1^{ss}$$

$$\frac{\partial f_1}{\partial x_2} = 0 \qquad \frac{\partial f_1}{\partial x_3} = 0 \qquad \frac{\partial f_1}{\partial x_4} = 0$$

$$\frac{\partial f_2}{\partial x_1} = k_1$$

$$\frac{\partial f_2}{\partial x_2} = -u_1^{ss} - k_2 \qquad \frac{\partial f_2}{\partial x_3} = 0 \qquad \frac{\partial f_2}{\partial x_4} = 0$$

$$\frac{\partial f_3}{\partial x_1} = 0 \qquad \frac{\partial f_3}{\partial x_2} = +k_2 \qquad \frac{\partial f_3}{\partial x_3} = -u_1^{ss} \qquad \frac{\partial f_3}{\partial x_4} = 0$$

$$\frac{\partial f_4}{\partial x_1} = \frac{1}{2} \cdot 2 k_3 x_1^{ss} \qquad \frac{\partial f_4}{\partial x_2} = -u_1^{ss} \qquad \frac{\partial f_4}{\partial x_3} = 0 \qquad \frac{\partial f_4}{\partial x_4} = 0$$

$$\begin{bmatrix} -u_1^{ss} - k_1 - 2k_3 x_1^{ss} & 0 & 0 & 0 \\ k_1 & -u_1^{ss} - k_2 & 0 & 0 \\ 0 & k_2 & -u_1^{ss} & 0 \\ k_3 x_1^{ss} & 0 & 0 & -u_1^{ss} \end{bmatrix}$$

$x_1^{ss} = 3$ mol/lt
$x_2^{ss} = 1.117$ mol/lt
$x_3^{ss} = 3.258$ mol/lt
$x_4^{ss} = 1.3125$ mol/lt
$u_1^{ss} = \frac{4}{7}$ min^{-1}
$u_2^{ss} =$

u_1^{ss}
$(x_1, x_2, x_3, x_4)^{ss}$

$k_1 = 5/6$
$k_2 = 5/3$
$k_3 = 1/6$

$C_{A1}^{ss} = 10$ mol/lt

$$\begin{bmatrix} \overbrace{10-3}^{B} & 10 \\ -1.117 & 0 \\ -3.258 & 0 \\ \cancel{-1.114} \; -1.3125 & 0 \end{bmatrix}$$

$$\frac{\partial f_1}{\partial x_1} = \frac{\partial f_1}{\partial (C_{A1} - C_A)} = \frac{\partial f_1}{\partial C_A} = -\frac{F^{ss}}{V} - K_1 - 2K_3 C_A^{ss} \qquad A_{11}$$

$$\frac{\partial f_1}{\partial x_2} = \frac{\partial f_1}{\partial (C_{B1} - C_B)} = \frac{\partial f_1}{\partial C_B} = 0 \qquad A_{12}$$

$$\frac{\partial f_2}{\partial x_1} = \frac{\partial f_2}{\partial (C_{Ai} - C_A)} = \frac{\partial f_2}{\partial C_A} = K_1 \qquad A_{21}$$

$$\frac{\partial f_2}{\partial x_2} = \frac{\partial f_2}{\partial (C_{Bi} - C_B)} = \frac{\partial f_2}{\partial C_B} = -F^{ss}/V - K_2 \qquad A_{22}$$

$$\frac{\partial f_1}{\partial u_1} = \frac{\partial f_1}{\partial (F/V - F^{ss}/V)} = \frac{\partial f_1}{\partial (F/V)} = C_{AF}^{ss} - C_A^{ss} \qquad B_{11}$$

$$\frac{\partial f_2}{\partial u_1} = \frac{\partial f_2}{\partial (F/V - F^{ss}/V)} = \frac{\partial f_2}{\partial (F/V)} = -C_{Bs} \qquad B_{21}$$

WE OBTAIN THE FOLLOWING SYSTEM MATRICES

$$A = \begin{bmatrix} -F/V - K_1 - 2K_3 C_A^{ss} & 0 \\ K_1 & -F^s/V - K_2 \end{bmatrix}$$

$$B = \begin{bmatrix} C_{AF}^{ss} - C_A^{ss} \\ -C_{Bs} \end{bmatrix}$$

The matrices can be particularised by considering different steady state operating points

CASE 1

CASE 2

CASE 3

$K_1 = 5/6$
$K_2 = 5/3$
$K_3 = 1/6$

$C_A^{ss} = 3$ mol/lt
$C_B^{ss} = 1.140$ mol/lt
$C_C^{ss} = 3.2580$ mol/lt
$C_D^{ss} = 1.3125$ mol/lt

$$\begin{array}{cc} -2.408 & -2.238 \end{array}$$

$$\overbrace{\begin{bmatrix} -4/7 - 5/6 - 2\cdot 1/6 \cdot 3 & 0 & 0 & 0 \\ 5/6 & -4/7 - 5/3 & 0 & 0 \\ 0 & 5/3 & -4/7 & 0 \\ 1/6 \cdot 3 & 0 & 0 & -4/7 \end{bmatrix}}^{A}$$

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$$\frac{\partial f_1}{\partial u_1} = \overset{u_2}{C_{Ai}} - x_1$$

$$\frac{\partial f_2}{\partial u_1} = -x_2$$

$$\frac{\partial f_3}{\partial u_1} = -x_3$$

$$\frac{\partial f_4}{\partial u_1} = -x_4$$

$$B = \begin{bmatrix} \overset{u_2^{ss}}{C_{Ai}^{ss}} - X_1^{ss} & u_1^{ss} \\ -X_2^{ss} & 0 \\ -X_3^{ss} & 0 \\ -X_4^{ss} & 0 \end{bmatrix}$$

$X_1^{ss} = 3$ mol/lt

$X_2^{ss} - 1.114$ mol/lt

$X_3^{ss} = 3.258$ mol/lt

$X_4^{ss} = 1.3125$ mol/lt

$u_1^{ss} = 4/7$

$C_{A1}^{ss} = 10$ mol/lt

$u_2^{ss} = 10$

$$\frac{\partial f_1}{\partial u_2} = u_1$$

$$\frac{\partial f_2}{\partial u_2} = 0$$

$$\frac{\partial f_3}{\partial u_2} = 0$$

$$\frac{\partial f_4}{\partial u_2} = 0$$