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Process Dynamics – CPN321

Semester Test 1

Chemical Engineering
Engineering and the Built Environment

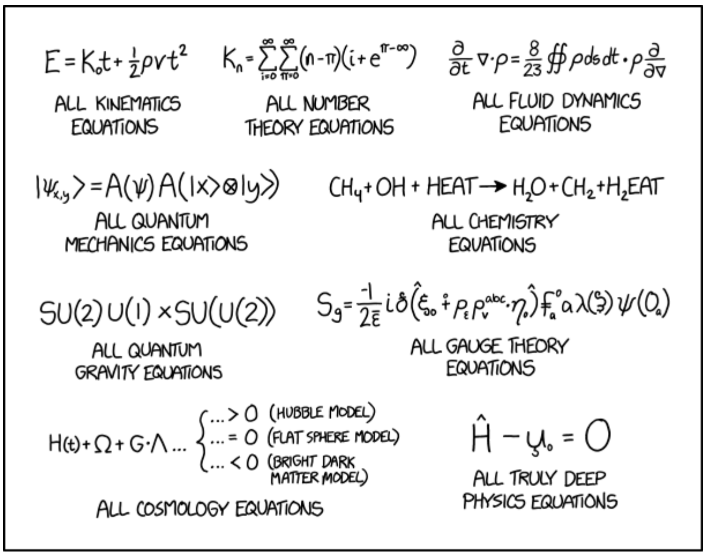
Examiner: Carl Sandrock

Date: 2018-03-13

Duration: 90 minutes   Total: 50   Total Pages: 10

Instructions – Read carefully

• Answer all the questions. • This is a closed book test. All the information you may use is contained in the paper. • You may use the computer • Make sure that you motivate all your answers and write legibly.



xkcd.com

1 Modelling

Irreversible consecutive reactions A $\xrightarrow{k_1}$ B $\xrightarrow{k_2}$ C occur in a jacketed, stirred-tank reactor as shown in Figure 1.

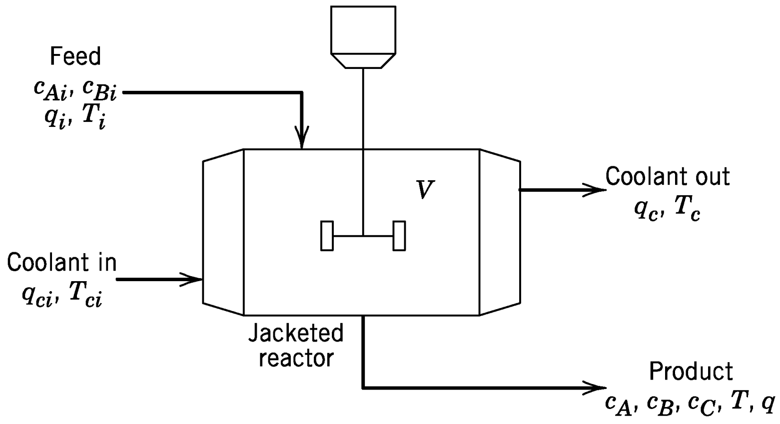


Figure 1: Jacketed tank reactor

On the plant, the coolant flow rate q_{ci} is manipulated to control the reactor temperature T, while the flow rate of the feed is manipulated in order to control the final product concentration c_C. The controller relations are not part of this question. The feed contains only A and B.

Additional information:

- The contents of the tank and cooling jacket are well mixed. The volumes of the material in the jacket and in the tank do not vary with time.
- The reaction rates are given by

$$r_1 = k_1 \exp\left(\frac{-E_1}{RT}\right) c_A \quad r_2 = k_2 \exp\left(\frac{-E_2}{RT}\right) c_B$$

  in units of $\mathrm{mol} \cdot \mathrm{h}^{-1} \cdot \mathrm{L}^{-1}$

- The thermal capacitances of the tank contents and the jacket ontents are significant relative to the thermal capacitances of the jacket and tank walls, which can be neglected.
- Constant pure component physical properties and heat transfer coefficients can be assumed.
- All flow rates are volumetric and given in $\mathrm{L} \cdot \mathrm{h}^{-1}$. The concentrations have units of $\mathrm{mol} \cdot \mathrm{L}^{-1}$. The heats of reaction are ΔH_1 and ΔH_2

Derive a dynamic model of the system and fill out the attached table. Make sure you classify all the symbols in your model as parameters, inputs and outputs and verify that the simulation problem is correctly specified for this system.

Total for question 1: $\boxed{30}$

2 Simulation

Answer this question on ClickUP

Find the values of x, y and z at the steady state of the following equations

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \sigma \cdot (y(t)^2 - x(t)) + u(t) \tag{1}$$

$$\frac{\mathrm{d}y}{\mathrm{d}t} = -x(t)z(t) + rx(t) - \ln(y(t)) \tag{2}$$

$$\frac{\mathrm{d}z}{\mathrm{d}t} = x(t)y(t) - bz(t) \tag{3}$$

With

$$r = 28 \qquad \sigma = 10 \qquad b = 3 \qquad u(t) = 1$$

It is known that the answer lies close to $\bar{x} = 20, \bar{y} = 5, \bar{z} = 30$

Total for question 2: *10*

3 Transfer function

Answer this question on ClickUP

For this question, assume that $\bar{x} = 20, \bar{y} = 5, \bar{z} = 30$ regardless of your answer for the previous quesiton.

After linearisation and expressed in terms of deviation variables, the previous equations become

$$\frac{\mathrm{d}x'}{\mathrm{d}t} = -\sigma x'(t) + 2\sigma\bar{y}y'(t) + u'(t) \tag{4}$$

$$\frac{\mathrm{d}y'}{\mathrm{d}t} = (r - \bar{z})x'(t) - \bar{x}z'(t) - y'(t)/\bar{y} \tag{5}$$

$$\frac{\mathrm{d}z'}{\mathrm{d}t} = \bar{y}x'(t) + \bar{x}y'(t) - bz'(t) \tag{6}$$

3.1. Equation 6 can be Laplace transformed and written as $-5x'(s) - 20y'(s) + \beta z'(s) = 0$. Find β. $\boxed{4}$

3.2. It can be shown that

$$\frac{Z(s)}{U(s)} = \frac{as + b}{s^3 + cs^2 + ds + e}$$

find the numeric values of a, b, c, d and e. $\boxed{6}$

Hint: you may find `sympy.solve` useful in this question.

Total for question 3: *10*

Full Marks $\boxed{50}$

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www.latex-project.org

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Datasheet: CPN321/CPB410

Compiled on May 5, 2018

General solution of 1st order DE:

$$\dot{x} + P(t)x = Q(t) \quad \Rightarrow \quad x = \frac{1}{F_I}\int Q(t)F_I\mathrm{d}t + c_1 \quad \text{with} \quad F_I = \exp\left(\int P(t)\mathrm{d}t\right)$$

Taylor Series expansion near point $x = a$:

$$f(x) = \sum_{n=0}^{\infty} \frac{f^n(a)}{n!}(x-a)^n$$

$$f(x_1,\ldots,x_d) = \sum_{n_1=0}^{\infty}\cdots\sum_{n_d=0}^{\infty} \frac{(x_1-a_1)^{n_1}\cdots(x_d-a_d)^{n_d}}{n_1!\cdots n_d!}\left(\frac{\partial^{n_1+\cdots+n_d}f}{\partial x_1^{n_1}\cdots\partial x_d^{n_d}}\right)(a_1,\ldots,a_d)$$

Linear approximation around point $\mathbf{x} = \mathbf{0}$, where $f(\mathbf{x}) = \mathbf{0}$:

$$f(\mathbf{x}) \approx \nabla f(\mathbf{0})\cdot\mathbf{x}$$

$$f(x_1,x_2,\cdots,x_d) \approx \frac{\partial f}{\partial x_1}(0)x_1 + \frac{\partial f}{\partial x_2}(0)x_2 + \cdots + \frac{\partial f}{\partial x_d}(0)x_d$$

Partial fraction expansion (for strictly proper rational functions of s)

$$F(s) = \frac{(s-z_1)(s-z_2)(s-z_3)\cdots}{(s-p_1)^n(s-p_2)(s-p_3)\cdots} = \underbrace{\sum_{m=0}^{n-1}\frac{A_m}{(s-p_1)^{n-m}}}_{\text{repeated roots}} + \frac{B}{s-p_2} + \frac{C}{s-p_3}\cdots$$

$$A_m = \lim_{s\to p_1}\left\{\frac{\mathrm{d}^m}{\mathrm{d}s^m}\Big[(s-p_1)^nF(s)\Big]\right\}\frac{1}{m!}$$

$$B = \lim_{s\to p_2}\big[(s-p_2)F(s)\big]$$

Euler identity:

$$e^{i\theta} = \cos\theta + i\sin\theta \quad \therefore e^{-i\theta} = \cos\theta - i\sin\theta \quad \text{and} \quad e^{i\pi} - 1 = 0$$

(1,1) Padé approximation of dead time:

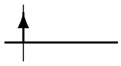
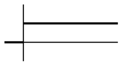
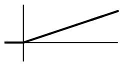
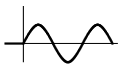
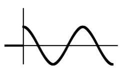
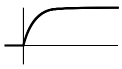
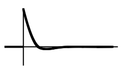
$$e^{-Ds} \approx \frac{1-\frac{D}{2}s}{1+\frac{D}{2}s}$$

PID controller:

$$m = K_C\left(\varepsilon + \frac{1}{\tau_I}\int_0^t \varepsilon\mathrm{d}t + \tau_D\frac{\mathrm{d}\varepsilon}{\mathrm{d}t}\right) \qquad \frac{m}{\varepsilon}(s) = K_C\left(1 + \frac{1}{\tau_I s} + \tau_D s\right)$$

Tuning rules:

	Ziegler-Nichols			Cohen-Coon (with $\phi = \frac{t_D}{\tau_P}$)		
	K_C	τ_I	τ_D	K_C	τ_I	τ_D
P	$\frac{K_u}{2}$			$\frac{\phi+3}{3K_P\phi}$		
PI	$\frac{K_u}{2.2}$	$\frac{P_u}{1.2}$		$\frac{5\phi+54}{60K_P\phi}$	$t_D\frac{30+3\phi}{9+20\phi}$	
PID	$\frac{K_u}{1.7}$	$\frac{P_u}{2}$	$\frac{P_u}{8}$	$\frac{3\phi+16}{12K_P\phi}$	$t_D\frac{32+6\phi}{13+8\phi}$	$\frac{4t_D}{11+2\phi}$

Time domain	Laplace-transform	z-transform ($b = e^{-aT}$)
Impulse: $\delta(t)$ 	1	1
Unit step: $u(t)$ 	$\frac{1}{s}$	$\frac{1}{1 - z^{-1}}$
Ramp: t 	$\frac{1}{s^2}$	$\frac{Tz^{-1}}{(1 - z^{-1})^2}$
t^n 	$\frac{n!}{s^{n+1}}$	$\lim_{a \to 0} (-1)^n \frac{\partial^n}{\partial a^n} \frac{1}{1 - bz^{-1}}$
e^{-at} 	$\frac{1}{s + a}$	$\frac{1}{1 - bz^{-1}}$
te^{-at} 	$\frac{1}{(s + a)^2}$	$\frac{Tbz^{-1}}{(1 - bz^{-1})^2}$
$t^2 e^{-at}$ 	$\frac{2}{(s + a)^3}$	$\frac{T^2 bz^{-1}(1 + bz^{-1})}{(1 - bz^{-1})^3}$
$\sin(\omega t)$ 	$\frac{\omega}{s^2 + \omega^2}$	$\frac{z^{-1} \sin(\omega T)}{1 - 2z^{-1} \cos(\omega T) + z^{-2}}$
$\cos(\omega t)$ 	$\frac{s}{s^2 + \omega^2}$	$\frac{1 - z^{-1} \cos(\omega T)}{1 - 2z^{-1} \cos(\omega T) + z^{-2}}$
$1 - e^{-at}$ 	$\frac{a}{s(s + a)}$	$\frac{(1 - b)z^{-1}}{(1 - z^{-1})(1 - bz^{-1})}$
$e^{-at} \sin(\omega t)$ 	$\frac{\omega}{(s + a)^2 + \omega^2}$	$\frac{z^{-1} b \sin(\omega T)}{1 - 2z^{-1} b \cos(\omega T) + b^2 z^{-2}}$
$e^{-at} \cos(\omega t)$ 	$\frac{s + a}{(s + a)^2 + \omega^2}$	$\frac{1 - z^{-1} b \cos(\omega T)}{1 - 2z^{-1} b \cos(\omega T) + b^2 z^{-2}}$
Initial value theorem: $\lim_{t \to 0} f(t)$	$\lim_{s \to \infty} sF(s)$	$\lim_{z \to \infty} F(z)$
Final value theorem: $\lim_{s \to \infty} f(t)$	$\lim_{s \to 0} sF(s)$	$\lim_{z \to 1} \left[\left(1 - z^{-1}\right) F(z) \right]$
Translation: $f(t - D)u(t - D)$	$e^{-Ds} F(s)$	$F(z) z^{-n}$ where $D = nT$
Derivative: $\frac{\mathrm{d}^n f(t)}{\mathrm{d}t^n} = f^n(t)$	$s^n F(s) - \sum_{k=1}^{n} s^{k-1} f^{n-k}(0)$	
Integral: $\int_0^t f(t) \mathrm{d}t$	$\frac{1}{s} F(s)$	
Zero$^{\text{th}}$ order hold	$H(s) = \frac{1 - e^{-Ts}}{s}$	