nonlinear process dynamics[1-5]

References:

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3. Seborg D.E., Mellichamp D. A., Edgar T.F, Doyle F.J., 2011, Process Dynamics and Control , John Wiley and Sons ISBN: 978-0-470-64610-6

4. Seborg D.E., Mellichamp D. A., Edgar T.F, Doyle F.J., ÇEVİRENLER: Tapan N.A., Erdoğan S. 3. baskıdan çeviriden 1.basım, 2012, Proses Dinamiği ve Kontrolu, Nobel Akademik Yayıncılık ISBN: 978-605-133-298-7

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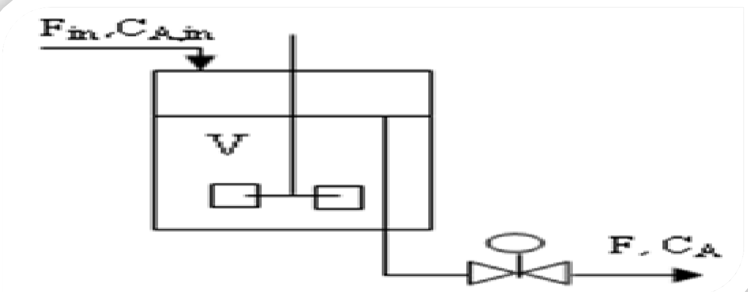
nonlinear reaction



$$\frac{d(C_A V)}{dt} = F_{in}C_{A,in} - FC_A - kC_A^{0.5}V$$

$$V\frac{dC_A}{dt} = FC_{A,in} - FC_A - kC_A^{0.5}V$$

$$FC_A = \overline{F}\overline{C}_A + (F-\overline{F})\overline{C}_A + (C_A-\overline{C}_A)\overline{F}$$

$$C_A^{0.5} = \overline{C}_A^{0.5} + (C_A-\overline{C}_A)(0.5\,\overline{C}_A^{-0.5})$$

$$V\frac{dC_A}{dt} = FC_{A,in} - \left[\overline{F}\overline{C}_A + (F-\overline{F})\overline{C}_A + (C_A-\overline{C}_A)\overline{F}\right] - kV\left[\overline{C}_A^{0.5} + (C_A-\overline{C}_A)(0.5\,\overline{C}_A^{-0.5})\right]$$

$$F' = F - \overline{F}$$

$$C'_A = C_A - \overline{C}_A$$

$$\longrightarrow \quad V\frac{dC'_A}{dt} = FC_{A,in} - \left[\overline{F}\overline{C}_A + F'\overline{C}_A + C'_A\overline{F}\right] - kV\left[\overline{C}_A^{0.5} + C'_A(0.5\,\overline{C}_A^{-0.5})\right] \quad \longrightarrow \quad 0 = \overline{F}C_{A,in} - \overline{F}\overline{C}_A - kV\overline{C}_A^{0.5}$$

$$V\frac{dC'_A}{dt} = F'C_{A,in} - F'\overline{C}_A - C'_A\overline{F} - C'_A(0.5\,kV\overline{C}_A^{-0.5}) \quad \longrightarrow \quad V\frac{dC'_A}{dt} + (\overline{F} + 0.5\,kV\overline{C}_A^{-0.5})C'_A = F'(C_{A,in} - \overline{C}_A)$$

$$\frac{V}{(\overline{F} + 0.5\,kV\overline{C}_A^{-0.5})}\frac{dC'_A}{dt} + C'_A = F'\frac{(C_{A,in} - \overline{C}_A)}{(\overline{F} + 0.5\,kV\overline{C}_A^{-0.5})} \quad \longrightarrow$$

$$\frac{V}{(\overline{F} + 0.5\,kV\overline{C}_A^{-0.5})}\,s\,C_A(s) + C_A(s) = F(s)\frac{(C_{A,in} - \overline{C}_A)}{(\overline{F} + 0.5\,kV\overline{C}_A^{-0.5})}$$

$$\left[\frac{V}{(\overline{F} + 0.5\,kV\overline{C}_A^{-0.5})}\,s + 1\right]C_A(s) = F(s)\frac{(C_{A,in} - \overline{C}_A)}{(\overline{F} + 0.5\,kV\overline{C}_A^{-0.5})}$$

Transfer Function:

$$\frac{C_A(s)}{F(s)} = \frac{\dfrac{(C_{A,in} - \bar{C}_A)}{(\bar{F} + 0.5\, kV\, \bar{C}_A^{-0.5})}}{\dfrac{V}{(\bar{F} + 0.5\, kV\, \bar{C}_A^{-0.5})} s + 1} = \frac{K}{\tau s + 1}$$

$$K = \frac{(C_{A,in} - \bar{C}_A)}{(\bar{F} + 0.5\, kV\, \bar{C}_A^{-0.5})} \qquad \tau = \frac{V}{(\bar{F} + 0.5\, kV\, \bar{C}_A^{-0.5})}$$

$$K = \frac{q}{(q + 0.5kVC_A^{0^{-0.5}})} = 0.00282 \quad \tau = \frac{V}{(q + 0.5kVC_A^{0^{-0.5}})} = 2.82s$$

$$0.00282\, C_{A0}^{'} = C_A^{'} + 2.82\frac{dC_A^{'}}{dt}$$

$$0.00282\, C_{A0}^{'}(s) = C_A^{'}(s) + 2.82sC_A^{'}(s) - C_A^{'}(0)$$

$$0.00282\, C_{A0}^{'}(s) = C_A^{'}(s)[2.82s + 1]$$

$$\frac{C_A^{'}(s)}{C_{A0}^{'}(s)} = \frac{0.00282}{[2.82s + 1]}$$

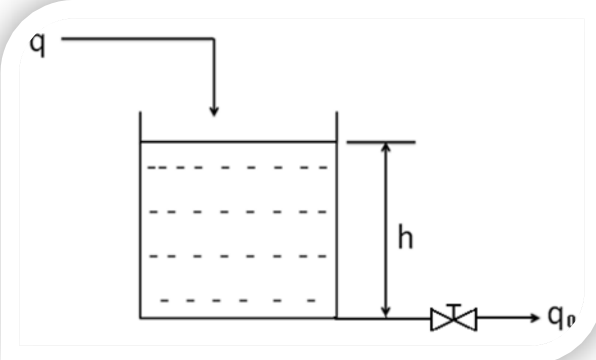
$$C'_{A0}(s) = \frac{1}{s}$$

$$C'_A(s) = \frac{0.00282}{[2.82s+1]}\frac{1}{s} = \frac{0.001}{s(s+0.355)} = \frac{A}{s} + \frac{B}{s+0.355}$$

$$A = 0.00282 \qquad B = -0.00282$$

$$C'_A(s) = \frac{0.00282}{s} - \frac{0.00282}{s+0.355}$$

$$C'_A(t) = 0.00282\left(1 - e^{-0.355t}\right)$$



$$q_0 = Ch^3$$

A liquid level system has a cross-sectional area of 0.2 m^2

Steady state $\quad q_s - q_{0_s} = 0 \quad \rightarrow \quad q_s - Ch_s^3 = 0$

Unsteady state $\quad q - q_0 = A\frac{dh}{dt} \quad \rightarrow \quad q - Ch^3 = A\frac{dh}{dt}$

Linearizing the nonlinear term, h^3, by means of a Taylor series expansion;

$$f(x) = f(x_s) + \left.\frac{df}{dx}\right|_{x_s} (x - x_s) + (higher\ order\ terms)$$

$$h^3 = h_s^3 + 3h_s^2(h - h_s)$$

Substituting the linearized term into unsteady state equation;

Unsteady state $q - C(h_s^3 + 3h_s^2(h - h_s)) = A\frac{dh}{dt}$

Unsteady state - Steady state $(q - q_s) - C(h_s^3 + 3h_s^2(h - h_s) - h_s^3) = A\frac{d(h-h_s)}{dt}$

$$(q - q_s) - 3Ch_s^2(h - h_s) = A\frac{d(h-h_s)}{dt}$$

Introducing deviation variables;

$$q - q_s = Q \quad ; \quad h - h_s = H$$

$$Q - 3Ch_s^2 H = A\frac{dH}{dt}$$

$$A\frac{dH}{dt} + 3Ch_s^2 H = Q$$

$$\frac{A}{3Ch_s^2}\frac{dH}{dt} + H = \frac{1}{3Ch_s^2}Q$$

$$\tau\frac{dH}{dt} + H = RQ$$

Taking the Laplace transform;

$$\tau[sH(s) - H(0)] + H(s) = RQ(s)$$

$$H(0) = h(0) - h_s = 0$$

$$\tau sH(s) + H(s) = RQ(s)$$

$$(\tau s + 1)H(s) = RQ(s)$$

$$\frac{H(s)}{Q(s)} = \frac{R}{\tau s + 1}$$

$$q_{0_s} = Ch_s^3$$

$$0.55\ \frac{m^3}{min} = C(1.5\ m)^3$$

$$C = 0.16\ \frac{1}{min}$$

$$\tau = \frac{A}{3Ch_s^2} = \frac{0.2\ m^2}{(3)(0.16\ \frac{1}{min})(1.5\ m)^2} \quad \rightarrow \quad \tau = 0.19\ min$$

$$R = \frac{1}{3Ch_s^2} = \frac{1}{(3)(0.16\ \frac{1}{min})(1.5\ m)^2} \quad \rightarrow \quad R = 0.93\ \frac{min}{m^2}$$

$$0.19\frac{dH}{dt} + H = 0.93\ Q$$

$$Q(t) = 0.85 - 0.55 = 0.3\ \frac{m^3}{min}$$

$$Q(s) = \frac{0.3}{s}$$

$$\frac{H(s)}{Q(s)} = \frac{0.93}{0.19\ s + 1}$$

$$H(s) = Q(s)\ \frac{0.93}{0.19\ s + 1}$$

$$H(s) = \left(\frac{0.3}{s}\right)\left(\frac{0.93}{0.19\ s + 1}\right) = \frac{0.28}{s(0.19s + 1)} = \frac{\frac{0.28}{0.19}}{s(s + \frac{1}{0.19})} = \frac{1.47}{s(s + 5.26)}$$

$$H(s) = \frac{1.47}{s(s + 5.26)} = \frac{A}{s} + \frac{B}{s + 5.26}$$

$$A = \left[\frac{1.47\ s}{s(s + 5.26)}\right]_{s=0} = 0.28$$

$$B = \left[\frac{1.47\ (s + 5.26)}{s(s + 5.26)}\right]_{s=-5.26} = -0.28$$

$$H(s) = \frac{0.28}{s} - \frac{0.28}{s+5.26} = 0.28\left[\frac{1}{s} - \frac{1}{s+5.26}\right]$$

Inverting to time domain;

$$H(t) = 0.28\,[1 - e^{-5.26t}]$$

$$H(t) = h(t) - h_s$$

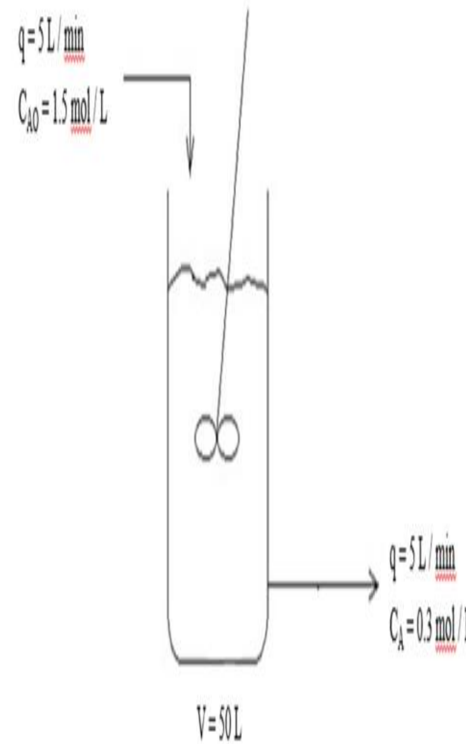
$$h(t) = h_s + H(t) \;\; \rightarrow \;\; h = 1.5 + 0.28\,[1 - e^{-5.26t}]$$

$$t = 3\,\text{min} \quad \rightarrow \;\; h(3) = 1.5 + 0.28\,[1 - e^{-5.26*3}]$$

$$h(3) = 1.78\,m$$

Consider the stirred-tank reactor shown below. The reaction occuring is $2A \rightarrow B$ and proceeds at a rate $-r_A = kC_A^2$, k = 1.8 (L/mol min)

Assuming constant density and constant volume.



Steady state $\quad qC_{AO_s} - qC_{A_s} + r_A V = 0 \quad \rightarrow \quad qC_{AO_s} - qC_{A_s} - kC_{As}^2 V = 0$

Unsteady state $\quad qC_{AO} - qC_A + r_A V = V\frac{dC_A}{dt} \quad \rightarrow \quad qC_{AO} - qC_A - kC_A^2 V = V\frac{dC_A}{dt}$

Linearizing the nonlinear term, C_A^2, by means of a Taylor series expansion;

$$f(x) = f(x_s) + \left.\frac{df}{dx}\right|_{x_s}(x - x_s) + (higher\ order\ terms)$$

$$C_A^2 = C_{As}^2 + 2C_{A_s}(C_A - C_{A_s})$$

Substituting the linearized term into unsteady state equation;

Unsteady state

$$qC_{AO} - qC_A - kV\left(C_{As}^2 + 2C_{A_s}(C_A - C_{A_s})\right) = V\frac{dC_A}{dt}$$

Unsteady state - Steady state

$$q\left(C_{AO} - C_{AO_s}\right) - q\left(C_A - C_{A_s}\right) - kV\left(C_{As}^2 + 2C_{A_s}(C_A - C_{A_s}) - C_{As}^2\right) = V\frac{dC_A}{dt}$$

$$q\left(C_{AO} - C_{AO_s}\right) - q\left(C_A - C_{A_s}\right) - 2kVC_{A_s}\left(C_A - C_{A_s}\right) = V\frac{d\left(C_A - C_{A_s}\right)}{dt}$$

Introducing deviation variables;

$$C_{AO} - C_{AO_s} = C'_{AO} \quad ; \quad C_A - C_{A_s} = C'_A$$

$$q\, C'_{AO} - qC'_A - 2kVC_{A_s}C'_A = V\frac{dC'_A}{dt}$$

$$V\frac{dC'_A}{dt} + C'_A\,(q + 2kVC_{A_s}) = qC'_{AO}$$

$$\frac{V}{q + 2kVC_{A_s}}\frac{dC'_A}{dt} + C'_A = \frac{q}{q + 2kVC_{A_s}}C'_{AO}$$

$$\tau\frac{dC'_A}{dt} + C'_A = RC'_{AO}$$

$$\tau = \frac{V}{q + 2kVC_{A_s}} \qquad R = \frac{q}{q + 2kVC_{A_s}}$$

Taking the Laplace transform;

$$\tau[s\, C'_A(s) - C'_A(0)] + C'_A(s) = R\, C'_{AO}(s)$$

$$C'_A(0) = C_A(0) - C_{A_s} = 0$$

$$\tau sC'_A(s) + C'_A(s) = R\, C'_{AO}(s)$$

$$(\tau s + 1)\, C'_A(s) = RC'_{AO}(s)$$

$$\frac{C'_A(s)}{C'_{AO}(s)} = \frac{R}{\tau s + 1}$$

$$\tau = \frac{V}{q + 2kVC_{A_s}} = \frac{50\ L}{\left(5\,\frac{L}{min}\right) + 2\ \left(1.8\ \frac{L}{mol\ min}\right)(50\ L)\left(0.3\,\frac{mol}{L}\right)} = 0.85\ min$$

$$R = \frac{q}{q + 2kVC_{A_s}} = \frac{5\ L/min}{\left(5\,\frac{L}{min}\right) + 2\ \left(1.8\ \frac{L}{mol\ min}\right)(50\ L)\left(0.3\,\frac{mol}{L}\right)} = 0.08$$

$$\frac{C_A^{'}(s)}{C_{AO}^{'}(s)} = \frac{0.08}{0.85s + 1}$$

$$C_{AO}^{'}(t) = \begin{Bmatrix} 1.5 & t < 0 \\ (4.0 - 1.5) & 0 \leq t < 1 \\ 1.5 & t \geq 1 \end{Bmatrix}$$

$$C_{AO}^{'}(t) = 2.5\,[\,u(t) - u(t-1)]$$

$$C_{AO}^{'}(s) = 2.5\ \left[\frac{1}{s} - \frac{1}{s}e^{-s}\right] = \frac{2.5}{s}[1 - e^{-s}]$$

$$\frac{C_A^{'}(s)}{C_{AO}^{'}(s)} = \frac{0.08}{0.85s + 1}$$

$$C_A^{'}(s) = C_{AO}^{'}(s)\frac{0.08}{0.85s + 1}$$

$$C_A^{'}(s) = \frac{2.5}{s}[1 - e^{-s}]\frac{0.08}{0.85s + 1}$$

$$C_A^{'}(s) = 0.2\ \frac{1}{s\,(0.85s + 1)}(1 - e^{-s}) = \frac{0.2}{s\,(0.85s + 1)} - \frac{0.2\ e^{-s}}{s\,(0.85s + 1)}$$

$$F(s) = \frac{0.2}{s\,(0.85s+1)} = \frac{0.24}{s\,(s+1.18)} = \frac{A}{s} + \frac{B}{s+1.18}$$

$$A = \frac{0.24}{s\,(s+1.18)}\,s = 0.20 \quad (s=0)$$

$$B = \frac{0.24}{s\,(s+1.18)}\,(s+1.18) = -0.20 \quad (s=-1.18)$$

$$F(s) = \frac{0.2}{s\,(0.85s+1)} = \frac{0.2}{s} - \frac{0.2}{s+1.18} \qquad F(t) = 0.2 - 0.2\,e^{-1.18\,t}$$

Translation of function $L\,\{f\,(t-t_o)\} = e^{-st_o} f(s)$

$$G(s) = \frac{0.2\,e^{-s}}{s\,(0.85s+1)} = \frac{0.24\,e^{-s}}{s\,(s+1.18)} \qquad G(t) = 0.2 - 0.2\,e^{-1.18(t-1)}$$

$$C'_A\,(t) = F(t) - G(t)$$

$$C'_A\,(t) = [0.2 - 0.2\,e^{-1.18\,t}] - [0.2 - 0.2\,e^{-1.18(t-1)}]$$

$$C'_A\,(t) = -0.2\,e^{-1.18\,t} + 0.2\,e^{-1.18(t-1)}$$

$$C'_A\,(t) = 0.2\,e^{-1.18\,t}(e^{1.18} - 1) = 0.45\;\; e^{-1.18\,t}$$

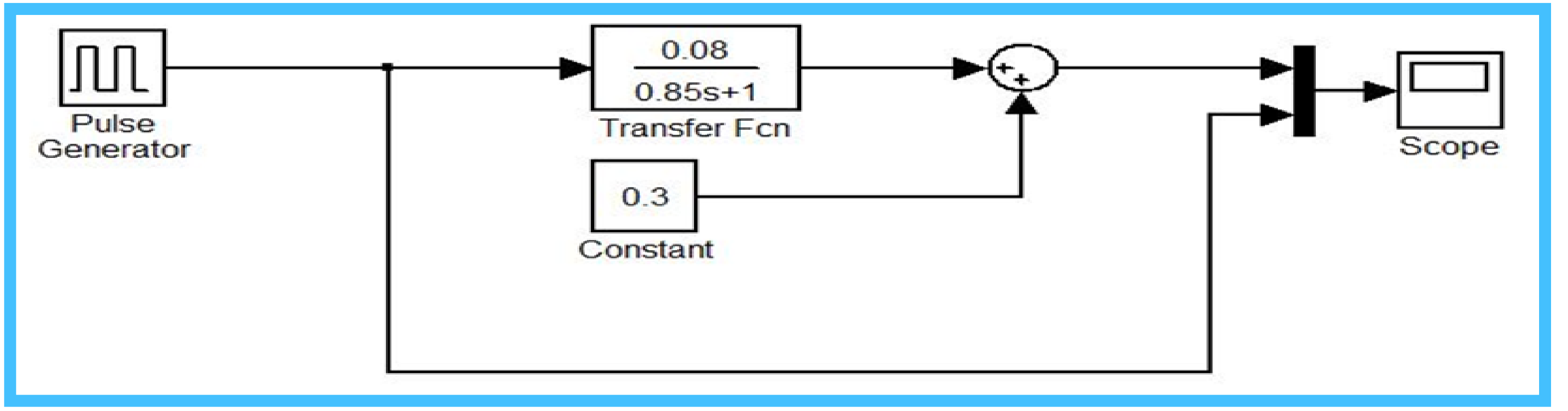
$$C'_A\,(t) = C_A\,(t) - C_{A_s}$$

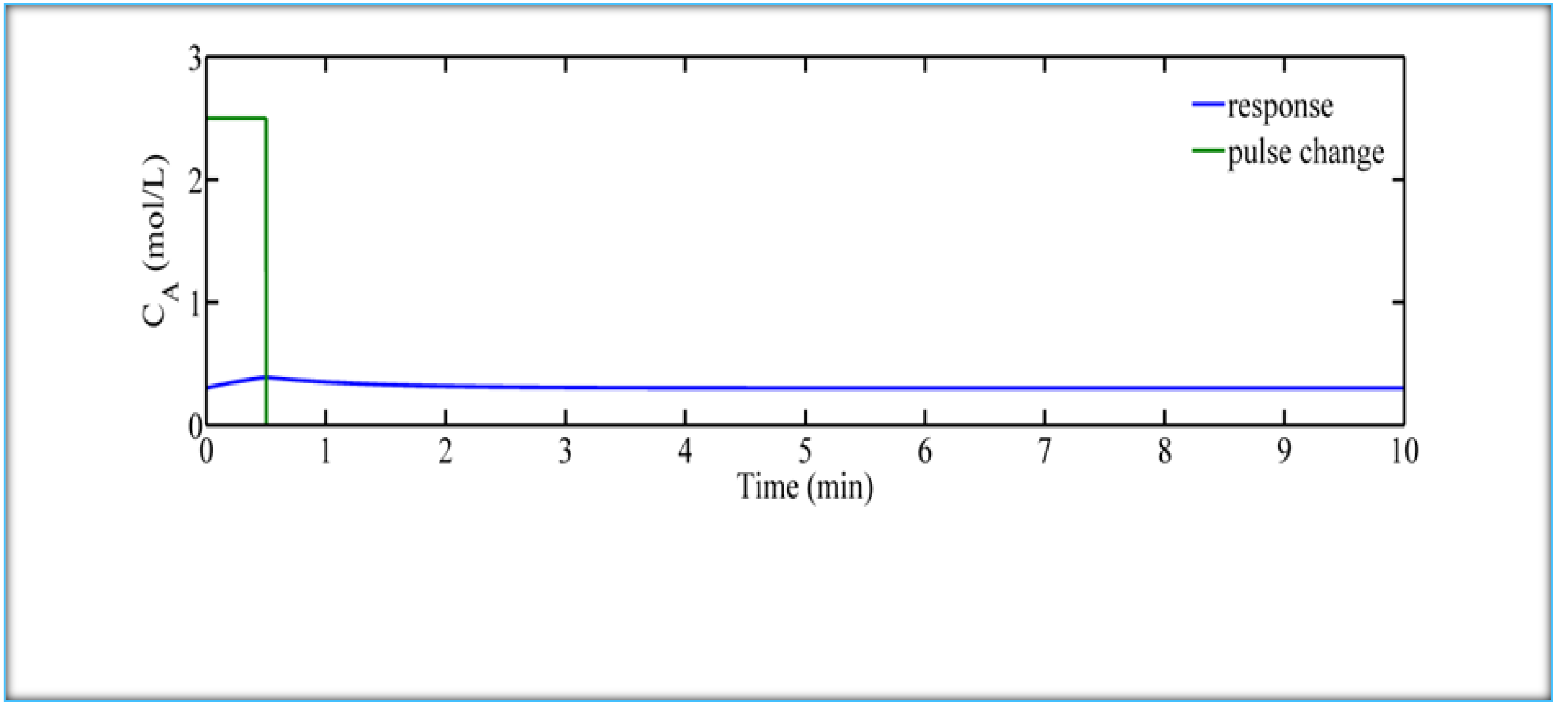
$$C_A\,(t) = C_{A_s} + C'_A\,(t)$$

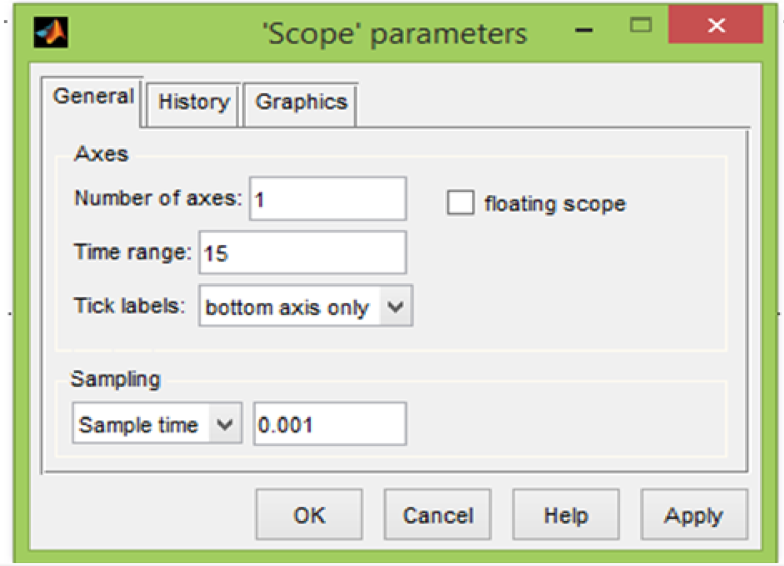
$$C_A\,(t) = 0.3 + 0.45\;\; e^{-1.18\,t}$$

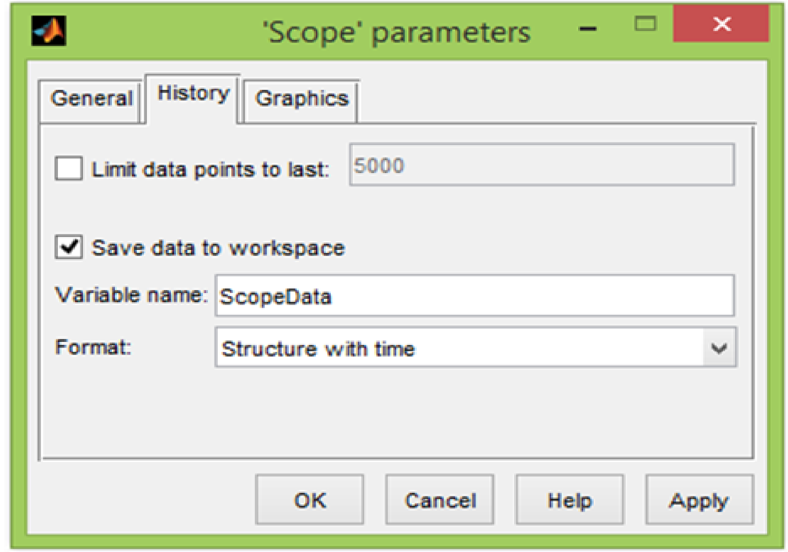
$t = 2$ min; $\quad C_A\,(2) = 0.3 + 0.45\;\; e^{-1.18*2} = 0.34\,mol/L$

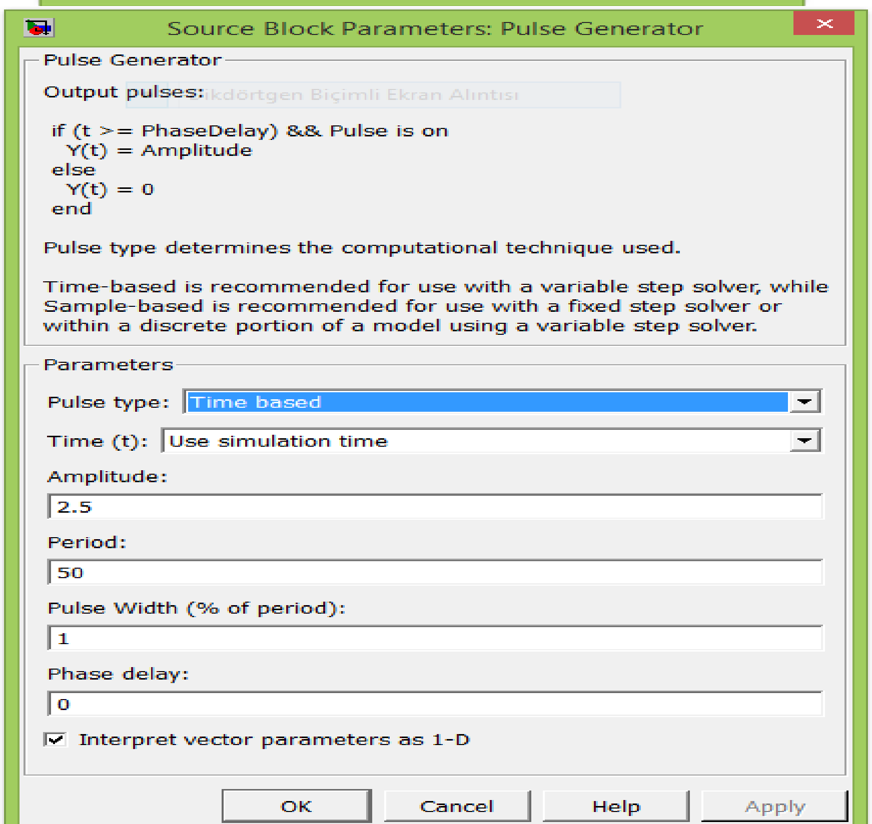
$t \to \infty$; $\qquad C_A\,(\infty) = 0.3 + 0.45\;\; e^{-1.18*0} = 0.3\,mol/L$

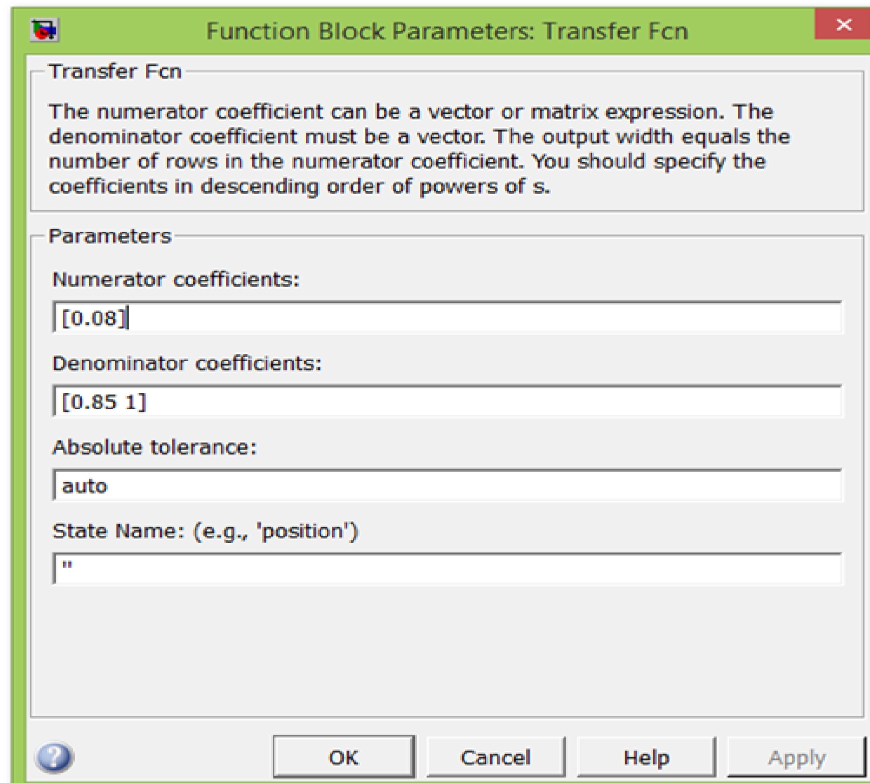

Pulse
Generator
0.08
0.85s+1
Transfer Fcn
0.3
Constant
Scope


response
pulse change
C_A (mol/L)
Time (min)
0
1
2
3
4
5
6
7
8
9
10


'Scope' parameters
General
History
Graphics
Axes
Number of axes: 1
floating scope
Time range: 15
Tick labels: bottom axis only
Sampling
Sample time
0.001
OK
Cancel
Help
Apply


'Scope' parameters
General
History
Graphics
Limit data points to last: 5000
Save data to workspace
Variable name: ScopeData
Format: Structure with time
OK
Cancel
Help
Apply


Source Block Parameters: Pulse Generator
Pulse Generator
Output pulses:
if (t >= PhaseDelay) && Pulse is on
Y(t) = Amplitude
else
Y(t) = 0
end
Pulse type determines the computational technique used.
Time-based is recommended for use with a variable step solver, while Sample-based is recommended for use with a fixed step solver or within a discrete portion of a model using a variable step solver.
Parameters
Pulse type: Time based
Time (t): Use simulation time
Amplitude:
2.5
Period:
50
Pulse Width (% of period):
1
Phase delay:
0
Interpret vector parameters as 1-D
OK
Cancel
Help
Apply


Function Block Parameters: Transfer Fcn
Transfer Fcn
The numerator coefficient can be a vector or matrix expression. The denominator coefficient must be a vector. The output width equals the number of rows in the numerator coefficient. You should specify the coefficients in descending order of powers of s.
Parameters
Numerator coefficients:
[0.08]
Denominator coefficients:
[0.85 1]
Absolute tolerance:
auto
State Name: (e.g., 'position')
''
OK
Cancel
Help
Apply