Scilab for Chemical Engineers

TSEC - Online Certificate Course

SAMPLE PROBLEMS

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XCOS

1 Mathematical Operations

1.1 Basic Arithmetic Operations in Chemical Reactions

Create an Xcos model to calculate the total moles of reactants given the quantities: 2 moles of Hydrogen (H_2) and 3 moles of Oxygen (O_2). Use addition and multiplication blocks to find the total moles.

1.2 Exponential Functions in Reaction Rates

Develop an Xcos model to evaluate the rate constant (k) of a first-order reaction using the Arrhenius equation: $k = Ae^{-E_a/RT}$. Define suitable values for pre-exponential factor (A), activation energy (E_a), gas constant (R), and temperature (T).

1.3 Logarithmic Functions in pH Calculation

Create an Xcos model to calculate the pH of a solution with a given hydrogen ion concentration $[H^+]$. Use the logarithm block to compute $pH = -\log([H^+])$.

1.4 Polynomial Evaluation in Thermodynamics

Construct an Xcos model to evaluate the specific heat capacity (Cp) of a substance as a function of temperature using the polynomial equation $Cp(T) = aT^2 + bT + c$. Define appropriate coefficients (a, b, c) and temperature (T) range.

1.5 Integration

Integrate the following data and plot the resulting function in xcos.

t	y
0.0	0.0000
0.5	0.4794
1.0	0.8415
1.5	0.9975
2.0	0.9093
2.5	0.5985
3.0	0.1411
3.5	-0.3508
4.0	-0.7568
4.5	-0.9775
5.0	-0.9589
5.5	-0.7055
6.0	-0.2794

Table 1: Discrete data points for integration using x-cos

Hint: Construct a `struct` with the keywords `struct_name.time` and `struct_name.values` and enter the data. These should strictly be column vectors!

1.6 Root finding using Graphical method 1

Using the graphical method, find the root of the following equation

$$f(t) = t^3 - 3t^2 - 3t + 1 \tag{1}$$

Hint: Split the function to $f_1(t) = t^3$ and $f_2(t) = 3t^2 + 3t - 1$. Shift the equations as there is no concept of negative time in xcos.

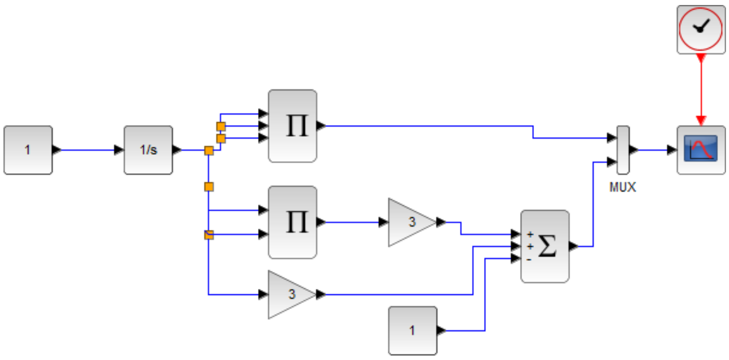

Figure 1: Finding the root of an equation

1.7 Root finding using Graphical method 2

Find the roots of the function using graphical method

$$f(t) = t^4 - 11t^2 + 2t + 1 \tag{2}$$

1.8 IVP: Ordinary Differential Equations 1

Solve the following ODE. Given initial condition $y(0) = 0$

$$\frac{\mathrm{d}y}{\mathrm{d}t} = t^2 - 3 \tag{3}$$

Compare with the analytical solution.

1.9 IVP: Ordinary Differential Equations 2

Solve the following ODE. Calculate the value of y at t = 1.4.

$$\frac{\mathrm{d}y}{\mathrm{d}t} = 3t^2 y \tag{4}$$

Consider the following initial conditions $y(t_0) = y(1) = 2$ *Hint*: You will have to shift these equations such that $y(0) = 2$. Go to `Set Context` menu and write `shift = 1`

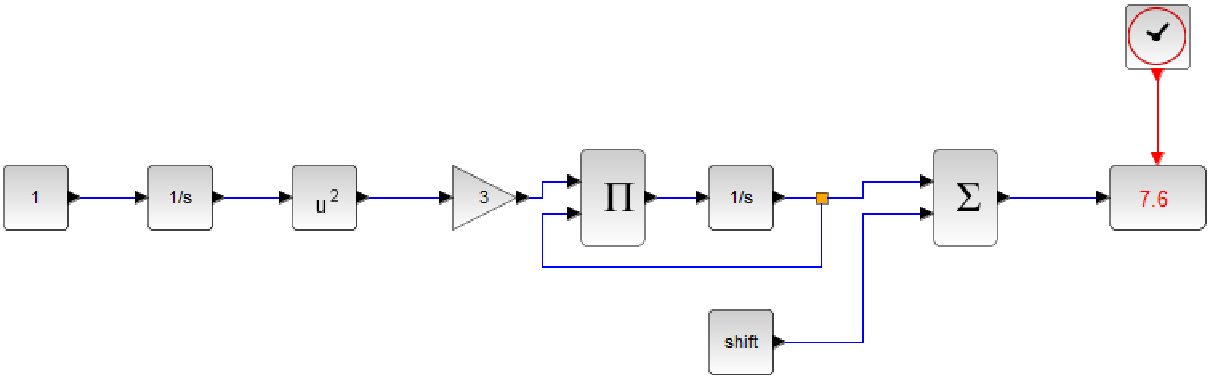

Figure 2: Solution to ODE

1.10 IVP: Ordinary Differential Equations 3

Solve the following ODE

$$\frac{\mathrm{d}y}{\mathrm{d}t} = y + t + yt \tag{5}$$

With the following initial conditions $y(0) = 1$

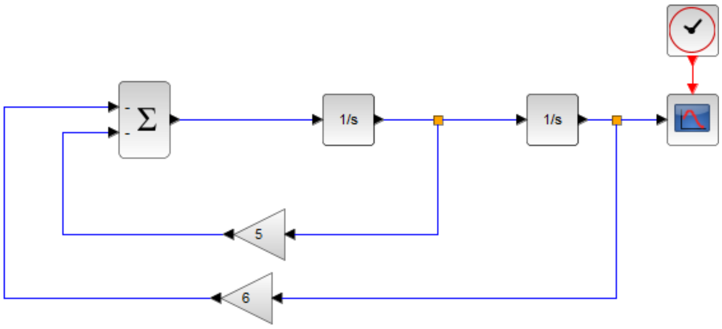

Figure 3: Second order ODE

1.11 Second order ODE

Solve the following second order ODE.

$$\frac{\mathrm{d}^2y}{\mathrm{d}t^2} + 5\frac{\mathrm{d}y}{\mathrm{d}t} + 6y = 0 \tag{6}$$

with the following initial conditions. $y'(0) = 1, y(0) = 0$. Simulate for $t = 4$ with $y_{\max} = 0.15$