

# SCILAB FOR CHEMICAL ENGINEERS

TSEC - ONLINE CERTIFICATE COURSE

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## PROJECTS

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ADITYA GANESH

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### Instructions

1. Every project has a link to the fundamentals that is required for solving it
2. Download this file to access the links
3. Every project has to be done individually
4. Animations are expected for your project
5. Write a report for your project as well (Preferably use  $\text{\LaTeX}$  to write your report. It is very easy to learn it by your own. Youtube link:  $\text{\LaTeX}$  for Students – A Simple Quickstart Guide)
6. Section 2 topics are reserved for second year students. These students can also attempt other projects
7. Name your files as  
`<Project_number>_<Year_of_study>_<Roll_no>_<Name>.<pdf/sce>`  
Example: 1.5\_3\_123456\_Aditya.pdf
8. If you have a project in mind and that is not listed, write an email to me describing your project in detail
9. My email id: 22D2017@iitb.ac.in
10. Attendance of 75% is mandatory to qualify for a certificate

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# 1 Process Simulation: Flowsheeting

Create a process flowsheet of a manufacturing unit using a scilab code. Basic mass conservation and component balance is expected. You can attempt energy conservation and/or dynamic flowsheeting if you want. Plot meaningful data.

For inspiration, have a look at these flowsheets: DWSIM Flowsheets

# 2 Fluid Dynamics: Trajectory of a particle

Write a scilab code to animate the trajectory of a particle in the following flows:

2.1 Extensional flow

2.2 Rotational flow

2.3 Sinusoidal flow

2.4 Oscillatory flow

2.5 Random flow (would resemble a turbulent flow case)

If possible, add more particles to the simulation.

# 3 Heat Transfer: Steady State Temperature Profile

Calculate the steady-state temperatures of the nodes in the figure below. The entire outer surface is exposed to the convection environment at  $20^{\circ}\text{C}$  and the entire inner surface is constant at  $500^{\circ}\text{C}$ . Assume  $k = 0.2 \text{ W/m}^{\circ}\text{C}$ . This time, pay attention to the varying  $dx$  in the domain. Write down the equations before numerically solving it.

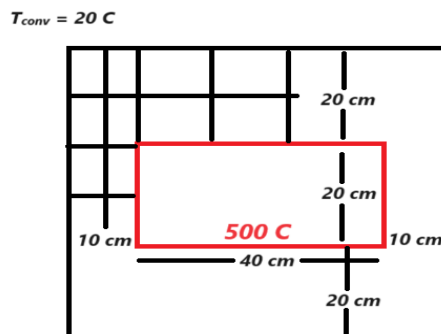


Figure 1: Heat transfer involving convection at the boundaries

Reference: Holman, J. P. (10th ed.). Heat Transfer (In S.I. Units). Tata McGraw-Hill Education. [Unsolved problem 3.56. Refer to table 3.2 in this book to understand how the numerical differentiation is done. This book also has programming examples towards the end].

## 4 Thermodynamics: NRTL Equation for multicomponent processes

The nonrandom, two-liquid (NRTL) equation was developed by Renon and Prausnitz to find the activity coefficients for multicomponent processes. Here we have a 4 components ( $C = 4$ ) which includes n-Heptane, Benzene, DMF and Water. The equation is given as:

$$\ln \gamma_i = \frac{\sum_{j=1}^C \tau_{ji} G_{ji} x_j}{\sum_{k=1}^C G_{ki} x_k} + \sum_{j=1}^C \left[ \frac{x_j G_{ij}}{\sum_{k=1}^C G_{kj} x_k} \left( \tau_{ji} - \frac{\sum_{k=1}^C x_k \tau_{kj} G_{kj}}{\sum_{k=1}^C G_{kj} x_k} \right) \right] \quad (1)$$

Where (case 1)  $x = [0.7895 \ 0.2105 \ 0 \ 0]$ ,

$$\tau = \begin{bmatrix} 0 & -0.355 & 1.910 & 4.806 \\ 1.196 & 0 & -0.240 & 3.639 \\ 2.036 & 0.676 & 0 & -2.128 \\ 7.038 & 5.750 & 2.506 & 0 \end{bmatrix} \quad \alpha = \begin{bmatrix} 0 & 0.300 & 0.250 & 0.150 \\ 0.300 & 0 & 0.425 & 0.203 \\ 0.250 & 0.425 & 0 & 0.253 \\ 0.150 & 0.203 & 0.253 & 0 \end{bmatrix} \quad (2)$$

And  $G_{ji} = \exp(-\alpha_{ji} \tau_{ji})$ . Write a Scilab code (all summation symbols refer to for loops) and/or directly calculate the activity coefficient of these four components using the data given above. Also test for (case 2)  $x = [0 \ 0.0909 \ 0.6818 \ 0.2273]$ . Divide the activity coefficients of (case 1) by (case 2). This will be termed as partition coefficient. To understand the significance of all these values, refer to the following book.

Reference: J. D. Seader, Ernest J. Henley, D. Keith Roper (5th Ed), Separation Process Principles with Applications Using Process Simulators (Solved Example 10.11)

## 5 Chaos Theory: The Rössler Attractor (or any other attractor of your choice, see ref.)

The Rössler system is another captivating example of chaotic behavior in a simple set of differential equations. It was first introduced by Otto Rössler as an accessible model for studying chaotic systems. The system exhibits complex and chaotic dynamics for specific parameter values and initial conditions. Like the Lorenz attractor, the Rössler attractor

also demonstrates sensitivity to initial conditions.

The Rössler equations describe the rate of change of three quantities with respect to time:

$$\frac{dx}{dt} = -y - z$$

$$\frac{dy}{dt} = x + ay$$

$$\frac{dz}{dt} = b + z(x - c)$$

Here,  $x, y, z$  represent the state variables,  $t$  denotes time, and  $a, b, c$  are system parameters that influence the behavior of the system. These are positive constants.

Solve these system of equations for the following initial conditions:

$$a = 0.2, \quad b = 0.2, \quad c = 5.7$$

Use a time step of  $dt = 0.01$ . For reference, check the following Youtube video.

YouTube video links:

- <https://www.youtube.com/watch?v=EXvLju3DLMY>
- Chaotic Attractors
- Rössler Attractor

## 6 Transport Phenomena: Laminar Flow Reactor

Consider fully developed flow in a circular pipe of a Newtonian fluid. The fluid has a soluble compound  $A$  at a concentration of  $C_{A0}$  at the inlet. This compound undergoes a chemical reaction in the system with a rate constant of  $k$ . The reaction is assumed to be of first order. Also, the walls are coated with a catalyst and the compound reacts at the wall with a surface reaction constant of  $k_s$ .

The differential equation for the concentration distribution of species A as a function of  $r$  and  $z$  as given by the convection–diffusion–reaction (CDR) model is

$$2\langle v \rangle \left( 1 - \left( \frac{r}{R} \right)^2 \right) \frac{\partial C_A}{\partial z} = D \left[ \frac{\partial^2 C_A}{\partial z^2} + \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial C_A}{\partial r} \right) \right] - k C_A \quad (3)$$

Upon non-dimensionalising these equations, we get [see ref. for further details]

$$2(1 - \xi^2) \frac{\partial c_A}{\partial \eta} = B \left[ \frac{1}{\xi} \frac{\partial}{\partial \xi} \left( \xi \frac{\partial c_A}{\partial \xi} \right) \right] - Da c_A \quad (4)$$

If the parameter B is small then the radial diffusion term can also be dropped, leading to a model called the pure convection model, which is also known as the segregated flow model. The segregated model has a simple representation:

$$2(1 - \xi^2) \frac{\partial c_A}{\partial \eta} = -Da c_A \quad (5)$$

This equation also has an analytical result.

$$c_A(\xi) = \exp \left( -\frac{Da\eta}{2(1 - \xi^2)} \right) \quad (6)$$

Solve Equation 5 using any numerical method (ODE) of your choice. You will have to solve this ODE multiple times for different values of  $\xi$  (at least 20 values excluding 1). At the inlet,  $\eta = 0$  and  $c_A = 1$ . Choose a  $Da$  value between 0 and 4. Compare your numerical result with your analytical result.

Also note, there is a singularity when  $\xi = 1$ . Use reference to overcome that singularity state. This means that you can vary  $\xi$  from 0 to 0.9, and then assume your boundary condition there for  $\xi = 1$ .

Since we will be having variable concentration towards the exit ( $\eta = 1$ ), it is good to represent our concentration values in terms of a cup-mixing averaged concentration. This is given by the equation

$$c_{A,b}(\eta) = 4 \int_0^1 \xi(1 - \xi^2) c_A(\xi) d\xi \quad (7)$$

Once you calculate your  $c_A$  values for all  $\xi$  at  $\eta = 1$ , use any numerical integration scheme to find this value. Compare it with the analytical solution

$$c_{A,b}(\eta = 1) = \frac{Da^2}{4} E.I.(Da/2) + (1 - Da/2) e^{-Da/2} \quad (8)$$

Where  $E.I.(Da/2)$  is the exponential integral function.

$$E.I.(z) = \frac{1}{2} \left( \log(z) - \log \left( \frac{1}{z} \right) \right) + \sum_{k=1}^{\infty} \frac{z^k}{k k!} + \gamma \quad (9)$$

Once you have setup your Scilab code for a particular  $Da$  value, vary the  $Da$  between  $[0, 4]$  and then plot  $c_{A,b}$  vs  $Da$ .

Reference: Ramachandran, P. A. (2014). Advanced transport phenomena: analysis, modeling, and computations. Cambridge University Press. (Problem 12.4)

## 7 Interfacial Engineering: Deformed water droplet

Consider a water bubble placed over a flat plate made up of stainless steel. This water bubble, which is initially stressed has now been relaxed. The governing equations are

$$\frac{\partial v_r}{\partial t} = \frac{F_R}{\rho} + \frac{2v_r^2}{r} \quad (10)$$

where  $v_r$  is the velocity of the droplet in the radial direction,  $F_R = 2\pi(r - R_E)\gamma_{SL}$  is the force acting due to surface tension,  $\rho$  is the density,  $r$  is the radial parameter,  $\gamma_{SL} = \gamma_S - \gamma_L \cos(\theta_E)$  is the surface tension between stainless steel and water, and

$$\frac{\partial r}{\partial t} = -v_r - \frac{\pi\gamma_{SL}r(r - R_E)}{v_r\rho} \quad (11)$$

Conservation of spherical cap volume gives us the following

$$R_E^3(2 + \cos \theta_E)(1 - \cos \theta_E)^2 = r^3(2 + \cos \theta)(1 - \cos \theta)^2 \quad (12)$$

The given conditions are

1.  $\gamma_S = 1.614 \text{ N/m}$
2.  $\gamma_L = 0.072 \text{ N/m}$
3.  $\theta_E = 71^\circ$
4.  $\theta_i = 30^\circ$
5.  $v_i = 1 \text{ mm/s}$
6.  $R_E = 2 \text{ mm}$
7.  $\rho = 1000 \text{ kg/m}^3$

Where the subscripts  $E$  indicate final values and  $i$  indicate initial values. Solve the system of differential equations and throw some insights on the problem. Such problems are called

as wetting/dewetting problems. Hint: You will also need  $r_i$  to solve the problem. Use Equation 12 for that. Use surface plots to get the spherical bubble shape. You may refer to the following animation: [GitHub animation](#)

## 8 Population Biology: Lotka–Volterra Competition Model

Here we have two species, sheeps and rabbits. Suppose that both species are competing for the same food supply (grass) and the amount available is limited. Furthermore, ignore all other complications, like predators, seasonal effects, and other sources of food. Then there are two main effects we should consider:

- Each species would grow to its carrying capacity in the absence of the other. This can be modeled by assuming logistic growth for each species. Rabbits have a legendary ability to reproduce, so they have a higher intrinsic growth rate.
- When rabbits and sheep encounter each other, trouble starts. Sometimes the rabbit gets to eat but more usually the sheep nudges the rabbit aside and starts nibbling (on the grass, that is). Assume that these conflicts occur at a rate proportional to the size of each population. (If there were twice as many sheep, the odds of a rabbit encountering the sheep would be twice as great.) Furthermore, assume that the conflicts reduce the growth rate for each species, but the effect is more severe for the rabbits.

A specific model that incorporates these assumptions is

$$\frac{dx}{dt} = x(3 - x - 2y) \quad (13)$$

$$\frac{dy}{dt} = y(2 - x - y) \quad (14)$$

where  $x(t)$  = population of rabbits,  $y(t)$  = population of sheep, and  $x, y \geq 0$ . For different initial conditions, prepare the phase-space portraits and time series data for the population of the rabbits and the sheeps. Document all possible situations in your report.

References:

- Strogatz, S. H. (2018). Nonlinear dynamics and chaos: with applications to physics, biology, chemistry, and engineering. CRC press. [Section 6.4]
- Mathematical fundamentals

- Predator-Prey Model
- Modelling Interspecific Competition
- Lotka-Volterra Equations

## 9 Systems Biology: Turing patterns

The Turing pattern is a fascinating concept introduced by English mathematician Alan Turing in his 1952 paper titled “The Chemical Basis of Morphogenesis.” It describes how natural patterns—such as stripes, spots, and other spatially periodic structures—can emerge autonomously from a uniform initial state. These patterns arise due to Turing instability, which results from the interplay between differential diffusion of chemical species and chemical reactions. Refer to the following video to replicate the results. Extend the model for a chemical engineering application.

Turing patterns: Reaction-Diffusion processes

## 10 Chemical Reaction Engineering: Catalytic Reactor

The elementary gas phase reaction  $2A \rightleftharpoons C$  is carried out in a packed bed reactor. There is a heat exchanger surrounding the reactor, and there is a pressure drop along the length of the reactor.

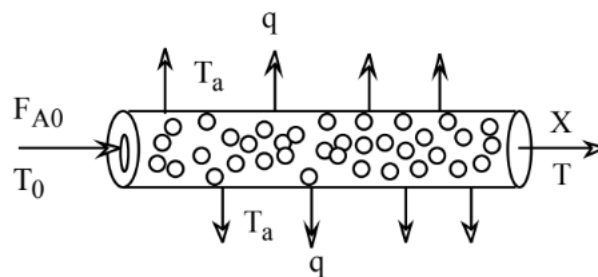


Figure 2: Packed Bed Catalytic Reactor

The various parameters values for this reactor design problem are summarized in Table 1.

1. Plot the conversion ( $X$ ), reduced pressure ( $y$ ) and temperature ( $T \times 10^{-3}$ ) along the reactor from  $W = 0$  kg up to  $W = 20$  kg.



Parameters	Value with units
$C_{PA}$	40.0 J/mol-K
$C_{PC}$	80.0 J/mol-K
$\Delta H_R$	-40,000 J/mol
$E_A$	41,800 J/mol-K
$k$	0.5 dm <sup>6</sup> /kg-min-mol @ 450 K
$K_C$	25,000 dm <sup>3</sup> /mol @ 450 K
$C_{A0}$	0.271 mol/dm <sup>3</sup>
$T_0$	450 K
$R$	8.314 J/mol-K
$F_{A0}$	5.0 mol/min
$UA$	0.8 J/kg-min-K
$T_a$	500 K
$\alpha$	0.015 kg <sup>-1</sup>
$P_0$	10 atm
$y_{A0}$	1.0 (Pure A feed)

Table 1: Parameter Values for Problem 10.

2. Around 16 kg of catalyst you will observe a “knee” in the conversion profile. Explain why this knee occurs and what parameters affect the knee.
3. Plot the concentration profiles for reactant  $A$  and product  $C$  from  $W = 0$  kg up to  $W = 20$  kg.

**Additional information:** The notation used here and the following equations and relationships for this particular problem are adapted from the textbook by Fogler. The problem is to be worked assuming plug flow with no radial gradients of concentrations and temperature at any location within the catalyst bed. The reactor design will use the conversion of  $A$  designated by  $X$  and the temperature  $T$  which are both functions of location within the catalyst bed specified by the catalyst weight  $W$ .

The general reactor design expression for a catalytic reaction in terms of conversion is a mole balance on reactant  $A$  given by

$$F_{A0} \frac{dX}{dW} = -r'_A \quad (15)$$

The simple catalytic reaction rate expression for this reversible reaction is

$$-r'_A = k \left[ C_A^2 - \frac{C_C}{K_C} \right] \quad (16)$$

where the rate constant is based on reactant  $A$  and follows the Arrhenius expression

$$k = k(@T = 450^\circ K) \exp \left( \frac{E_A}{R} \left[ \frac{1}{450} - \frac{1}{T} \right] \right) \quad (17)$$

and the equilibrium constant variation with temperature can be determined from van't Hoff's equation with  $\Delta\tilde{C}_P = 0$

$$K_C = K_C(@T = 450^\circ K) \exp \left( \frac{\Delta H_R}{R} \left[ \frac{1}{450} - \frac{1}{T} \right] \right) \quad (18)$$

The stoichiometry for  $2A \rightleftharpoons C$  and the stoichiometric table for a gas allow the concentrations to be expressed as a function of conversion and temperature while allowing for volumetric changes due to decrease in moles during the reaction. Therefore

$$C_A = C_{A0} \left( \frac{1-X}{1+\varepsilon X} \right) \frac{P}{P_0} \frac{T_0}{T} = C_{A0} \left( \frac{1-X}{1-0.5X} \right) y \frac{T_0}{T} \quad (19)$$

and

$$y = \frac{P}{P_0} \quad (20)$$

$$C_C = \left( \frac{0.5C_{A0}X}{1-0.5X} \right) y \frac{T_0}{T} \quad (21)$$

The pressure drop can be expressed as a differential equation (see Fogler for details)

$$\frac{d \left( \frac{P}{P_0} \right)}{dW} = \frac{-\alpha(1+\varepsilon X)}{2} \frac{P_0}{P} \frac{T}{T_0} \quad (22)$$

or

$$\frac{dy}{dW} = \frac{-\alpha(1-0.5X)}{2y} \frac{T}{T_0} \quad (23)$$

The general energy balance may be written as

$$\frac{dT}{dW} = \frac{UA(T_a - T) + r'_A(\Delta H_R)}{F_{A0} \left( \sum_i \theta_i C_{P,i} + X\Delta\tilde{C}_P \right)} \quad (24)$$

which for only reactant  $A$  in the reactor feed simplifies to

$$\frac{dT}{dW} = \frac{UA(T_a - T) + r'_A(\Delta H_R)}{F_{A0}C_{PA}} \quad (25)$$

Reference: Fogler, H. S. (6th Edition). Elements of chemical reaction engineering. Pearson Education.

## 11 Process Dynamics and Control: PID controller

A PID controller (Proportional–Integral–Derivative controller) is a widely used mechanism in industrial control systems and other applications requiring continuous modulation. Write a Scilab code and also a xcos simulation of a PID controller.

Reference: PID code website

## 12 Reactor Design: Catalyst selectivity

Consider a series reaction represented as  $A \rightarrow B \rightarrow C$  The governing equations are as follows.

$$\frac{d^2 c_A}{dx^2} = \phi_1^2 c_A \quad \frac{d^2 c_B}{dx^2} = -\phi_1^2 c_A + \phi_2^2 c_B \quad (26)$$

Here  $c$  is the dimensionless concentrations and the subscripts indicate the species;  $\phi$  is the Thiele modulus corresponding to the reaction. The boundary condition at  $x = 0$  (pore mouth) depends on the bulk concentrations of A and B (*Dirichlet*). The boundary condition at  $x = 1$  (pore end) is the no-flux condition (*Neumann*) for both A and B. The solution vector  $y$  has the size of four and consists of

$$y = \begin{bmatrix} y_1 = c_A \\ y_2 = \frac{dc_A}{dx} \\ y_3 = c_B \\ y_4 = \frac{dc_B}{dx} \end{bmatrix} \quad (27)$$

The system is now formulated as four first-order ODEs for the four components of the solution vector. Solve these equations for  $\phi_1 = 2$  and  $\phi_2 = 5$ . A key parameter of design interest is the yield of B, which is a measure of the rate of the reaction A to B compared with that for B to C. This is defined as the ratio of the flux of B outward from the surface to the flux of A into the surface:

$$\text{Yield of B} = - \left( \frac{dc_B/dx}{dc_A/dx} \right)_{x=1} \quad (28)$$

The initial conditions are  $c_A = 1$  and  $c_B = 0$ . The initial slopes are  $dc_A/dx = -\phi_1$  and  $dc_B/dx = 0$  (You may want to meddle here based on reference 1). In the present case the yield is equal to 0.0304. Try to maximize the yield by changing the Thiele modulus and report these values. The explanation is that if the size of the catalyst is small then B is able to diffuse out faster than it can react further, and hence the B to C reaction is reduced. The manipulation of the yield by choice of appropriate catalyst size and shape is an important inverse problem in reactor design.

References:

- Ramachandran, P. A. (2014). Advanced transport phenomena: analysis, modeling, and computations. Cambridge University Press. (Solved Example 10.9.2)
- YouTube video: Shooting method for converting 2nd order differential equations to 1st order differential equations