Chemical Engineering Applications in Scilab

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Introduction

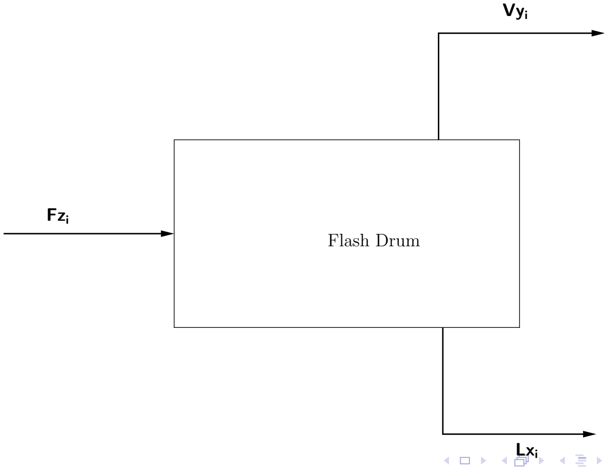
In Chemical Engineering the type of problems that occur are

- **Modeling and Simulation**
- **Parameter Estimation**
- **Determination of State variable (Steady State and non Steady State)**
- **Variation of Parameters**

Example: Flash Drum

Ref.:Patwardhan,S., Lecture notes

A three component mixture is fed to the Flash Drum It is operated at constant pressure and temperature



Contd.

We have following Equations

1. **Equilibrium Relations**

$$y_i = k_i x_i (i = 1, 2, 3)$$

2. **Overall Mass Balance**

$$F = L + V$$

3. **Component Balance**

$$Fz_i = Lx_i + Vy_i = Lx_i + Vk_i x_i$$

4. $$\sum x_i = 1$$

Contd.

- **Set of Non-linear Algebraic Equations**
- **We have 5 equations and 5 unknown**
- **Can be written as**

$$f_1(x_1, x_2, x_3, L, V) = 0$$

$$f_2(x_1, x_2, x_3, L, V) = 0$$

$$f_3(x_1, x_2, x_3, L, V) = 0$$

$$f_4(x_1, x_2, x_3, L, V) = 0$$

$$f_5(x_1, x_2, x_3, L, V) = 0$$

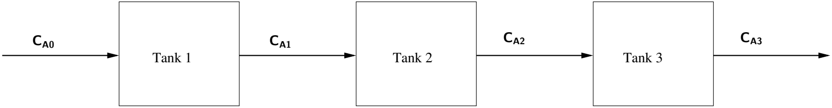
or

$$F(\bar{x}) = \bar{0}$$

Example: CSTR in Series

Ref.: Luyben,1990

Consider 3 CSTRs connected in series



Three CSTRs in Series (Open Loop)

By Mass Balance

$$dC_{A1}/dt = 1/\tau(C_{A0} - C_{A1}) - kC_{A_1}$$

$$dC_{A2}/dt = 1/\tau(C_{A1} - C_{A2}) - kC_{A_2}$$

$$dC_{A3}/dt = 1/\tau(C_{A2} - C_{A3}) - kC_{A_3}$$

Here

$$\tau = \nu/V$$

Contd.

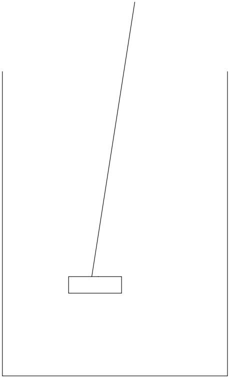
- **Set of differential equations**
- **To be solved simultaneously**
- **Scilab can be used**

Problem 1: Determination of specific reaction rate

Ref:Fogler,2004, Example4.1

- **Parameter Estimation Problem**
- **Experiment was conducted in batch reactor**
- **Equation for the reaction is**

$$\mathbf{A + B \rightarrow C}$$



Assumptions and Approximations

- **Assumptions**
  1. **Isothermal Conditions**
  2. **Zero order reaction**
  3. **Well mixed**
  4. **All reactants enters at the same time**
- **Approximation**
  1. **Reactant B is in excess so its concentration does not change**

Mathematical Formulation

The reaction rate

$$r_A = f(T, C_A)$$

reaction rate is given by

$$-r_A = -dC_A/dt = k_A C_A$$

$$\int_{C_{A0}}^{C_A} dC_A/C_A = -k_A \int_0^t dt$$

we get

$$\log(C_A/C_{A0}) = -k_A t$$

and Substituting

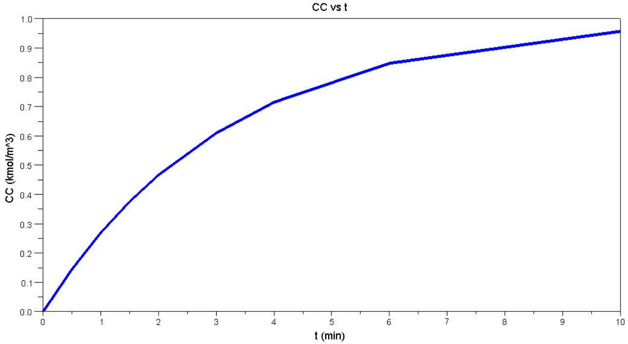
$$C_A = C_{A0} - C_c$$

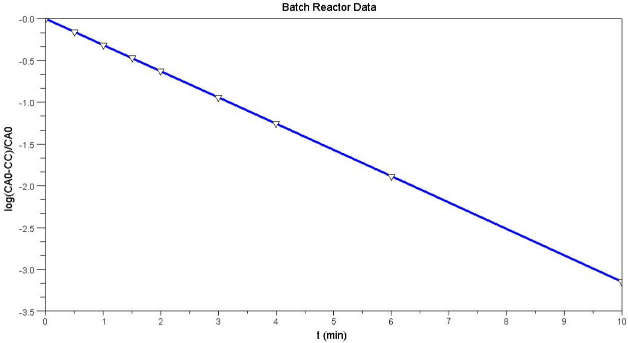
$$\log((C_{A0} - C_c)/(C_{A0})) = -k_A t$$

Data Analysis

Data has been given

1. **t**
2. **CA0**
3. **Cc**





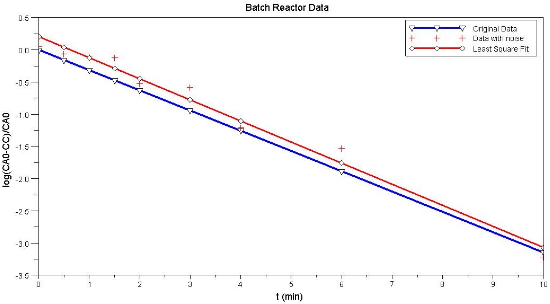
- **Slope**

$$k_A = -0.314 \text{min}^{-1}$$

- **Data is Exact**
- **Effect of noise on experimental data**

Effect of Noise

- **Add noise to the data (using random numbers)**
- **Calculate slope using First and Last data point**



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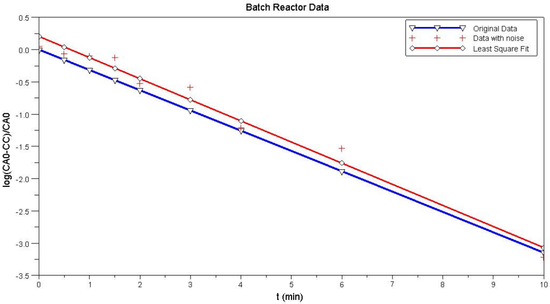

- **Apply Least Square Fit Analysis (Use reglin command in Scilab)**

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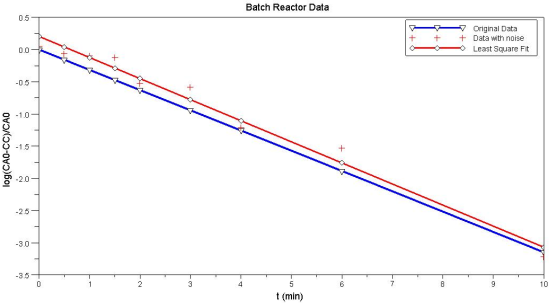

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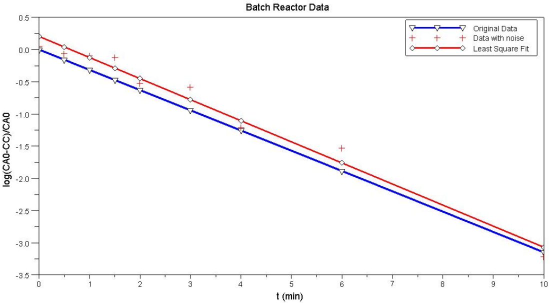
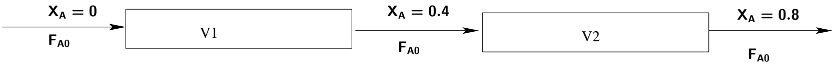


- **Apply Least Square Fit Analysis (Use reglin command in Scilab)**
- **Calculate slope using Points calculated by L.S. Fit**
- **Which slope is closer to the slope of original data ?**

Problem 2: Sizing Plug-Flow Reactors(PFRs) in Series

Ref:Fogler,2004, Example2.6

- **Variation of Parameter**
- **Two PFRs are connected in series**



Plug Flow Reactors in Series (Ref.:Fogler, 2004)

- **Total volume required for the given conversion**

Mathematical Formulation

Mass balance over elemental volume dV of the reactor

$$-r_A dV = F_{A0} dX_A$$

Rearranging and integrating

$$\int_0^V dV/F_{A0} = -\int_{X_{A1}}^{X_{A2}} dX_A/r_A$$

$$V = F_{A0} \int_{X_{A2}}^{X_{A1}} dX_A/r_A$$

There are two PFR's in series so

$$V_1 = F_{A0} \int_0^{X_{A1}} dX_A/r_A$$

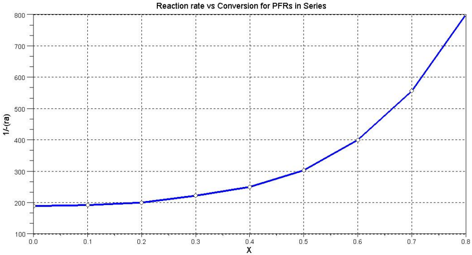
Contd..

and

$$V_2 = F_{A0} \int_{X_{A1}}^{X_{A2}} dX_A / r_A$$

Total Volume

$$V = V_1 + V_2$$



Role of Scilab

- **Need to integrate the above Equations**
- **Create a function file to integrate above equations**
- **Use help "inttrap" command in Scilab for integration**

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The results are

$$V_1 = 72.26 dm^3$$

$$V_2 = 154.67 dm^3$$

and

$$V = 226.93 dm^3$$

Problem 3: Air flow trough a straight pipe

Ref:McCabe, Smith, 1993, Example6.2
Data given

- **Entering air pressure, temperature and velocity**
- **Pipe diameter and length Assumptions**
- **Flow is isothermal**
- **Pressure at the discharge end is to be found**

Mathematical formulation

By mechanical energy balance

$$dp/\rho = d(u^2/2g_c) + (u^2/2g_c)fdL/r_H$$

$$\rho dp = \rho^2 d(u^2/2g_c) + \rho^2(u^2/2g_c)fdL/r_H$$

Also

$$u\rho = G$$

$$udu = -(G^2\rho^{-3})d\rho$$

and

$$\rho = Mp/RT$$

Contd.

On Substitution, we get

$$(M/RT)pdp - G^2/(g_c)d\rho/\rho + G^2 fdL/(2g_c r_H)$$

Integrating between stations a and b

$$(M/2RT)(p_a^2 - p_b^2) - G^2/(g_c)\ln \rho_a/\rho_b = G^2 f\Delta L/(2g_c r_H)$$

Using

$$p_a/p_b$$

in place of

$$\rho_a/\rho_b$$

and rearranging

$$p_b = \sqrt{p_a^2 - (2RT/M)G^2 f\Delta L/(2g_c r_H) + G^2/(g_c)\ln p_a/p_b}$$

Role of Scilab

- **Still a complicated expression**
- **Non-linear Algebraic Equation**
- **Create a function file to solve the above equation**
- **Use help "fsolve" to solve these equations**

Role of Scilab

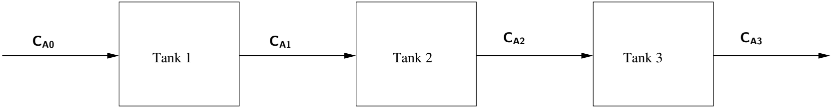
- **Still a complicated expression**
- **Non-linear Algebraic Equation**
- **Create a function file to solve the above equation**
- **Use help "fsolve" to solve these equations**
  Result is

$$p_a = 1.22 \text{bar}$$

Problem 4 : Continuous Stirrer Tank Reactors (CSTR) in Series (Open Loop)

Ref:Luyben,1990, Example5.2

- **3 CSTRs are connected in series**



Three CSTRs in Series (Open Loop)

- **Step change of 0.8 is applied at t = 0 to Tank 1**
- **Find out concentration profile in Tank 3**

Mathematical Formulation

- **Determination of State variable**
- **Making a Mass Balance over each tank, we get**

$$dC_{A1}/dt = 1/\tau(C_{A0} - C_{A1}) - kC_{A_1}$$

$$dC_{A2}/dt = 1/\tau(C_{A1} - C_{A2}) - kC_{A_2}$$

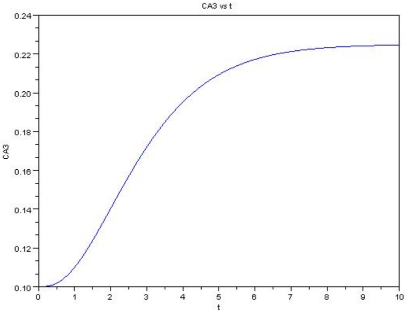
$$dC_{A3}/dt = 1/\tau(C_{A2} - C_{A3}) - kC_{A_3}$$

Here

$$\tau = \nu/V$$

Role of Scilab

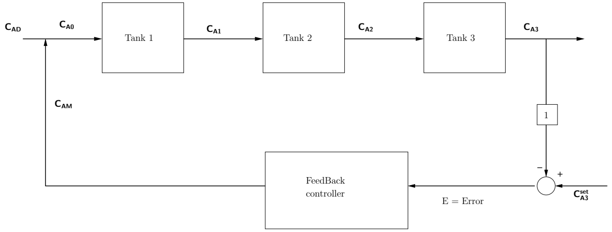
- **Use "ode" to solve set of differential equations**
- **Create a function file to solve the set of differential equations**



Problem 4(Extension): Continuous Stirrer Tank Reactors (CSTR) in Series (Closed Loop)

Ref:Luyben,1990, Example5.2

- **PI controller is added**



Closed Loop three-CSTR process (Ref.: Luyben)

- **Step change of 0.8 is applied at $t = 0$ to Tank 1**
- **Find out concentration profile in Tank 3**

mathematical Formulation

- **From the previous problem, we have**

$$\mathbf{dC_{A1}/dt = 1/\tau(C_{A0} - C_{A1}) - kC_{A_1}}$$

$$\mathbf{dC_{A2}/dt = 1/\tau(C_{A1} - C_{A2}) - kC_{A_2}}$$

$$\mathbf{dC_{A3}/dt = 1/\tau(C_{A2} - C_{A3}) - kC_{A_3}}$$

- **We have two more equations in this system**

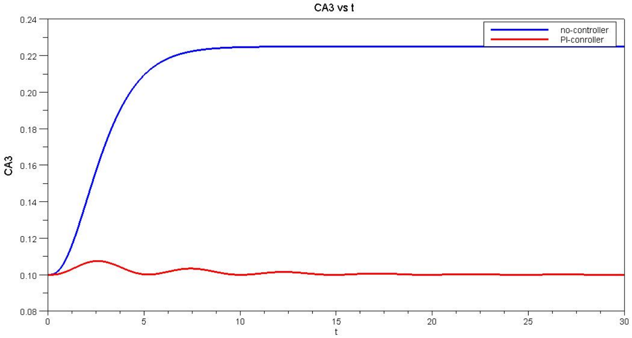
$$\mathbf{C_{A0} = C_{AD} + C_{AM}}$$

$$\mathbf{E = C_{A3}^{set} - C_{A3}}$$

$$\mathbf{C_{AM} = 0.8 + K_c(E + 1/\tau_I \int E_{(t)}dt)}$$

Role of Scilab

- **Use "ode" to solve set of differential equations**
- **Create a function file to solve the set of differential equations**



Concluding Remarks

- **Numerical techniques are available**
- **Does not have the data base (properties of gases, etc.)**
- **Work required in this direction**
- **Still a powerful tool for numerical and mathematical calculation**

References

1. **Patwardhan, S.,C., Lecture Notes for Computational Methods in Chemical Engineering**
2. **McCabe, L.,W., Smith, J.,C., Harriott, P., Unit Operations of Chemical Engineering, Fifth Edition, 1993**
3. **Fogler, H.,S., Elements of Chemical Reaction Engineering, Third Edition, 2004,**
4. **Luyben, W., L., Process Modeling, Simulation, and Control for Chemical Engineers, Second Edition, 1990**

Thank You.