

## Solutions to ODEs in Reaction Engineering

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(1) Solve the following ODEs for the given initial conditions:

(i)  $dx/dt = a x$  with  $x = x_o$  at  $t = 0$ .

Rearranging the above to integrate we get

$$\int \frac{dx}{x} = \int a dt$$

which gives

$$\ln x = a t + const$$

Since  $x = x_o$  at  $t = 0$ , we get  $const = \ln x_o$ . Therefore,

$$\ln x = a t + \ln x_o$$

which gives

$$\ln \left( \frac{x}{x_o} \right) = a t$$

and thus

$$x = x_o \exp(at)$$

(ii)  $dx/dt = a(1 + \epsilon x)$  with  $x = 0$  at  $t = 0$ .

Rearranging the above to integrate we get

$$\int \frac{dx}{1 + \epsilon x} = \int a dt$$

which gives

$$\frac{\ln(1 + \epsilon x)}{\epsilon} = a t + const$$

Since  $x = 0$  at  $t = 0$ , we get  $const = \ln(1)/\epsilon = 0$ . Therefore,

$$\frac{\ln(1 + \epsilon x)}{\epsilon} = a t$$

which gives

$$\ln(1 + \epsilon x) = a \epsilon t$$

and thus

$$x = \frac{\exp(a \epsilon t) - 1}{\epsilon}$$

(2) Solve the following ODEs for a non-zero value of  $\epsilon$  and give the solutions in terms of integrating constants:

(i)  $dx/dt = a [(1 - x)/(1 + \epsilon x)]$

Rearranging the above to integrate we get

$$\int \frac{1 + \epsilon x}{1 - x} dx = \int a dt$$

Substituting  $y = 1 - x$  gives  $x = 1 - y$  and  $dx = -dy$ , and hence the above expression becomes

$$\int -\frac{1 + \epsilon(1 - y)}{y} dy = \int a dt$$

which is rearranged to give

$$\int \left( -\frac{1 + \epsilon}{y} + \epsilon \right) dy = \int a dt$$

Upon integration of the above we get

$$-(1 + \epsilon) \ln y + \epsilon y = a t + \text{const}$$

Replacing the  $y$  in the above expression by  $(1 - x)$ , we get

$$-(1 + \epsilon) \ln(1 - x) + \epsilon(1 - x) = a t + \text{const}$$

(ii)  $dx/dt = a [(1 - x)^2/(1 + \epsilon x)]$

Rearranging the above to integrate we get

$$\int \frac{1 + \epsilon x}{(1 - x)^2} dx = \int a dt$$

Substituting  $y = 1 - x$  gives  $x = 1 - y$  and  $dx = -dy$ , and hence the above expression becomes

$$\int -\frac{1 + \epsilon(1 - y)}{y^2} dy = \int a dt$$

which is rearranged to give

$$\int \left( -\frac{1 + \epsilon}{y^2} + \frac{\epsilon}{y} \right) dy = \int a dt$$

Upon integration of the above we get

$$\frac{1 + \epsilon}{y} + \epsilon \ln y = a t + \text{const}$$

Replacing the  $y$  in the above expression by  $(1 - x)$ , we get

$$\frac{1 + \epsilon}{1 - x} + \epsilon \ln(1 - x) = a t + \text{const}$$

(iii)  $dx/dt = a [(1 - x)^2 / (1 + \epsilon x)^2]$

Rearranging the above to integrate we get

$$\int \frac{(1 + \epsilon x)^2}{(1 - x)^2} dx = \int a dt$$

Substituting  $y = 1 - x$  gives  $x = 1 - y$  and  $dx = -dy$ , and hence the above expression becomes

$$\int -\frac{(1 + \epsilon - \epsilon y)^2}{y^2} dy = \int a dt$$

which is rearranged to give

$$\int -\left(\frac{(1 + \epsilon)^2}{y^2} - \frac{2\epsilon(1 + \epsilon)}{y} + \epsilon^2\right) dy = \int a dt$$

Upon integration of the above we get

$$\frac{(1 + \epsilon)^2}{y} + 2\epsilon(1 + \epsilon) \ln y - \epsilon^2 y = a t + const$$

Replacing the  $y$  in the above expression by  $(1 - x)$ , we get

$$\frac{(1 + \epsilon)^2}{1 - x} + 2\epsilon(1 + \epsilon) \ln(1 - x) - \epsilon^2(1 - x) = a t + const$$

**(3)** Solve  $dx/dt = a(x - p)(x - q)$  and give the solutions in terms of integrating constants.

(i) For  $p \neq q$

Rearranging the above to integrate we get

$$\int \frac{dx}{(x - p)(x - q)} = \int a dt$$

which can be written as

$$\int \left(\frac{1}{p - q}\right) \left(\frac{1}{x - p} - \frac{1}{x - q}\right) dx = \int a dt$$

Upon integration we get

$$\left(\frac{1}{p - q}\right) (\ln(x - p) - \ln(x - q)) = a t + const$$

which is simply

$$\left(\frac{1}{p - q}\right) \ln\left(\frac{x - p}{x - q}\right) = a t + const$$

(ii) For  $p = q$

Rearranging the above to integrate we get

$$\int \frac{dx}{(x - p)^2} = \int a dt$$

Upon integration we get

$$\frac{-1}{x - p} = a t + const$$

(4) Solve  $dx/dt = (c + gx)/(a + bx)$  for the initial condition  $x = 0$  at  $t = 0$ .

Rearranging the above to integrate we get

$$\int \frac{a + bx}{c + gx} dx = \int dt$$

Substituting  $y = c + gx$  gives  $x = (y - c)/g$  and  $dx = dy/g$ , and hence the above expression becomes

$$\int \frac{a + b(y - c)/g}{gy} dy = \int dt$$

which is rearranged to give

$$\int \left( \frac{ag - bc}{g^2 y} + \frac{b}{g^2} \right) dy = \int dt$$

Upon integration of the above we get

$$\frac{ag - bc}{g^2} \ln y + \frac{b}{g^2} y = t + const$$

Replacing the  $y$  in the above expression by  $(c + gx)$ , we get

$$\frac{ag - bc}{g^2} \ln(c + gx) + \frac{b}{g^2}(c + gx) = t + const$$

Substituting the initial condition  $x = 0$  at  $t = 0$  in the above, we get

$$\frac{ag - bc}{g^2} \ln c + \frac{b}{g^2} c = const$$

Removing the *const* from the above two expressions by subtraction, we get

$$\frac{ag - bc}{g^2} \ln \left( \frac{c + gx}{c} \right) + \frac{b}{g} x = t$$

(5) Solve the following set of ODEs with the initial condition of  $C_A = C_{A0}$  and  $C_B = 0$  at  $t = 0$ :

$$\begin{aligned} \frac{dC_A}{dt} &= -k_1 C_A \\ \frac{dC_B}{dt} &= -k_2 C_B + k_1 C_A \end{aligned}$$

(i) For  $k_1 \neq k_2$

From the solution to part (i) of Problem (1) (see page 1), we could see that integrating the first ODE given above,

$$\frac{dC_A}{dt} = -k_1 C_A \quad (0.1)$$

with the initial condition of  $C_A = C_{A0}$  at  $t = 0$ , gives

$$C_A = C_{A0} \exp(-k_1 t) \quad (0.2)$$

Integrating the second ODE,

$$\frac{dC_B}{dt} = -k_2 C_B + k_1 C_A \quad (0.3)$$

is of course not straight forward since the above ODE has three variables, which are  $C_A$ ,  $C_B$  and  $t$ . Substituting (0.2) in (0.3), we get

$$\frac{dC_B}{dt} = -k_2 C_B + k_1 C_{Ao} \exp(-k_1 t) \quad (0.4)$$

in which  $C_B$  and  $t$  could not be separated. Therefore, we use the Integrating Factor method to integrate (0.4) as follows:

Rewrite (0.4) as

$$\frac{dC_B}{dt} + k_2 C_B = k_1 C_{Ao} \exp(-k_1 t)$$

Multiply the above equation by the Integrating Factor of the above equation, which is  $\exp(k_2 t)$ . We then get

$$\exp(k_2 t) \frac{dC_B}{dt} + \exp(k_2 t) k_2 C_B = \exp(k_2 t) k_1 C_{Ao} \exp(-k_1 t)$$

The left-hand-side of the above equation can be combined to give the following,

$$\frac{d}{dt} [\exp(k_2 t) C_B] = \exp(k_2 t) k_1 C_{Ao} \exp(-k_1 t)$$

which could be rewritten as

$$d [\exp(k_2 t) C_B] = k_1 C_{Ao} \exp[(-k_1 + k_2) t] dt \quad (0.5)$$

Upon integration (0.5) gives

$$\exp(k_2 t) C_B = \frac{k_1}{-k_1 + k_2} C_{Ao} \exp[(-k_1 + k_2) t] + const \quad (0.6)$$

Substituting the initial condition  $C_B = 0$  at  $t = 0$  in (0.6), we get

$$0 = \frac{k_1}{-k_1 + k_2} C_{Ao} + const \quad (0.7)$$

Subtracting (0.7) from (0.6), we get

$$\exp(k_2 t) C_B = \frac{k_1}{-k_1 + k_2} C_{Ao} \exp[(-k_1 + k_2) t] - \frac{k_1}{-k_1 + k_2} C_{Ao}$$

which could be rearranged to give

$$C_B = \frac{k_1}{-k_1 + k_2} C_{Ao} [\exp(-k_1 t) - \exp(-k_2 t)]$$

(ii) For  $k_1 = k_2$

If  $k_1 = k_2$ , then (0.5) could not be integrated to get (0.6). We must first substitute  $k_1 = k_2$  in (0.5). We then get

$$d[\exp(k_1 t) C_B] = k_1 C_{A_0} dt \quad (0.8)$$

Upon integration (0.8) gives

$$\exp(k_1 t) C_B = k_1 C_{A_0} t + \text{const} \quad (0.9)$$

Substituting the initial condition  $C_B = 0$  at  $t = 0$  in (0.9), we get

$$0 = \text{const}$$

Therefore, (0.9) gives

$$C_B = k_1 C_{A_0} t \exp(-k_1 t)$$