# Statistical and Numerical Methods for Chemical Engineers Solutions : Exercise 3

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## 1 Fixed Point Iterations

1. Show analytically that the three fixed point equations are consistent with (1) by rearranging the equations (2) to (4) to the form of (1).

$$f(x) = x\text{exp}(x) - 1 = 0 \tag{1}$$

$$x = \phi_1(x) \text{ with } \phi_1(x) = \text{exp}(-x) \tag{2}$$

$$x = \phi_2(x) \text{ with } \phi_2(x) = \frac{x^2\text{exp}(x) + 1}{\text{exp}(x)(1+x)} \tag{3}$$

$$x = \phi_3(x) \text{ with } \phi_3(x) = x + 1 - x\text{exp}(x) \tag{4}$$

First, for the second fixed point iteration $\phi_1(x)$, transposing $-1$ to the other side of the equation (1) gives

$$x\text{exp}(x) = 1 \tag{5}$$

By dividing by exp(x) on each side of the equation (5), we obtain the expression of the equation (2):

$$x = \text{exp}(-x) \tag{6}$$

For the second fixed point iteration $\phi_2(x)$, start by multiplying x to each side of equation (5):

$$x^2\text{exp}(x) = x \tag{7}$$

Add 1 to each side to get

$$x^2\text{exp}(x) + 1 = x + 1 \tag{8}$$

Using equation (5), equation (10) can be rearranged to

$$x^2\text{exp}(x) + 1 = (x+1)x\text{exp}(x) \tag{9}$$

Dividing by $(x+1)exp(x)$ gives the expression for equation (3) :

$$x = \frac{x^2\text{exp}(x) + 1}{\text{exp}(x)(1+x)} \tag{10}$$

For the second fixed point iteration $\phi_3(x)$, start from simple rearrangement of $x = x + 1 - 1$, where the final term 1 is substituted by $1 = xexp(x)$ from equation (5):

$$x = x + 1 - x\text{exp}(x) \tag{11}$$

which is the expression for the equation (4).

2. Solutions for questions 2 to 5 are provided in the attached mfile `SNM_Ex3_Q1.m`.

## 2 Linear Interpolation

Refer to the separately attached solution mfile `SNM_Ex3_Q2.m`.

## 3 System of Nonlinear Equations

Refer to the separately attached solution mfile `SNM_Ex3_Q3.m` and function mfiles `CSTRFun.m`, `CSTRJac.m`, `jacobianest.m`, and `newtonMethod.m`.