15CH305J Computational Techniques in Chemical Engineering

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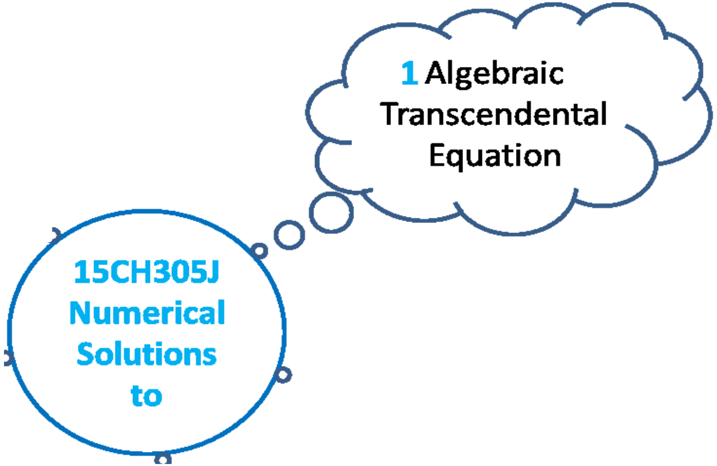
Unit 1 – Numerical (or iterative) solution to transcendental (or nonlinear) algebraic equations

- Review of iterative methods: Bisection, Regula-Falsi and Newton-Raphson methods
- Phase equilibrium problems and Equation of State
- Determination of Bubble and Dew points



Linear and Nonlinear equations

Given below is the van der Waal's equation of state:

$$\left(p + \frac{a}{v^2}\right)(v - b) = RT$$

Where v =*V*/*n* is molal volume (m^3/kmol); a and b are empirical constants, R = Universal gas constant and T is the temperature of the gas

Solving the above equation to determine p for a given v is easy while solving for v for specified values of p and T is relatively difficult.

What makes an equation *easy or difficult* to solve is its *linearity* or *non linearity* in the *unknown variable* ?

Linear and Nonlinear equations

Equations that contain *unknown variables raised to the first power only* (x but not x^2 or $x^{1/2}$) , and *that do not contains transcendental functions* (sin x, e^x) or products (x, y) of unknown variables, are called *Linear Equations.*

Equations that do not satisfy these conditions are called *nonlinear* equations

For example, if a, b, and b are constants, and x , y , and z are variables,

$ax + by = c$ is linear

$ax^2 = by + c$ is nonlinear (contains x^2)

$x - \ln(x) + b = 0$ is nonlinear contains $\ln(x)$

Linear and Nonlinear equations

A *single equation* containing *several variables* may be *linear* with respect to some variables and *nonlinear* with respect to others. For example

$$xy - e^{x} = 3$$

is *linear* in y and *nonlinear* in x. If x isknown, the equation may easily be solved for y, while the solution for x *from* a known variable of y is much *harder* to obtain.

$$P\hat{V} = RT\left(1 + \frac{B(T)}{\hat{V}} + \frac{C(T)}{\hat{V}^2}\right)$$

Linear and Nonlinear equations

Another example is the three-term virial equation of state:

$$P\hat{V} = RT\left(1 + \frac{B(T)}{\hat{V}} + \frac{C(T)}{\hat{V}^2}\right)$$

where *B* and *C* are known functions of temperature

This equation is linear in P and nonlinear in $\hat{v}$ and T. It is easy to solve for P *from* given values of T and $\hat{v}$ and difficult to solve for either $\hat{v}$ or T from given values of the other two variables.

Linear and Nonlinear equations

Linear equations that contain *a single unknown* variable have one and only one solution (*one root*).

For example

$$7x - 3 = 2x + 4 \Longrightarrow x = 1.2$$

$$\left.\begin{aligned} P\hat{V} &= RT \\ P = 3,\ R &= 2,\ T = 300 \end{aligned}\right\} \Longrightarrow \hat{V} = RT/P = (2)(300)/(3) = 200$$

Linear and Nonlinear equations

In contrast, *nonlinear equations* that contain *a single unknown va*riable may have *any number of real roots* (as well as *imaginary and complex* roots). For example,

$$x^2 + 1 = 0 \quad \text{has no real roots}$$
$$x^2 - 1 = 0 \quad \text{has two real roots } (x = +1 \text{ and } x = -1)$$
$$x - e^{-x} = 0 \quad \text{has one real root } (x = 0.56714\ldots)$$
$$\sin x = 0 \quad \text{has an infinite number of real roots } (x = 0, \pi, 2\pi, \ldots)$$

The roots of some nonlinear equations, such as the second of the equations given above, can be obtained directly using simple algebra, but most nonlinear equations must be solved using an *iterative or trial-and-error technique*.

Solution to nonlinear equation in single variable

- Graphical method
- Simple iterative procedure or successive approximation
- Bisection
- Regula falsi
- Newton Raphson method

Solution to nonlinear equation in single variable – ***Graphical Method***

- Graphical method is a simple method for obtaining root of the function $f(x) = 0$
- The procedure is, make a plot and observe where it crosses x –axis
- This point, represents the value x for which $f(x) = 0$ provides a *rough approximation* of the *root*

Solution to nonlinear equation in single variable – ***Iterative method***

- An iterative method is also called as "*trial and error*" method or successive approximation/fixed point iteration
- It is used to obtain *an estimate* of the function $f(x)$

Solution to nonlinear equation in single variable – Example problem on ***Graphical method***

- Problem : 1 Evaluate the square root of a positive number A i.e. $(\sqrt{A})$, where $A > 0$ by graphical method. Consider $A = 2$.

- From problem statement we have $x = \sqrt{A}$ (1)
- $(1) \Longrightarrow x = \sqrt{2}$ (2)
- The above equation (2) can be rewritten as

$$(2) \Longrightarrow x^2 = 2 \quad (3)$$

Equation (2) can be rearranged as

$$(3) \Longrightarrow f(x) = x^2 - 2$$

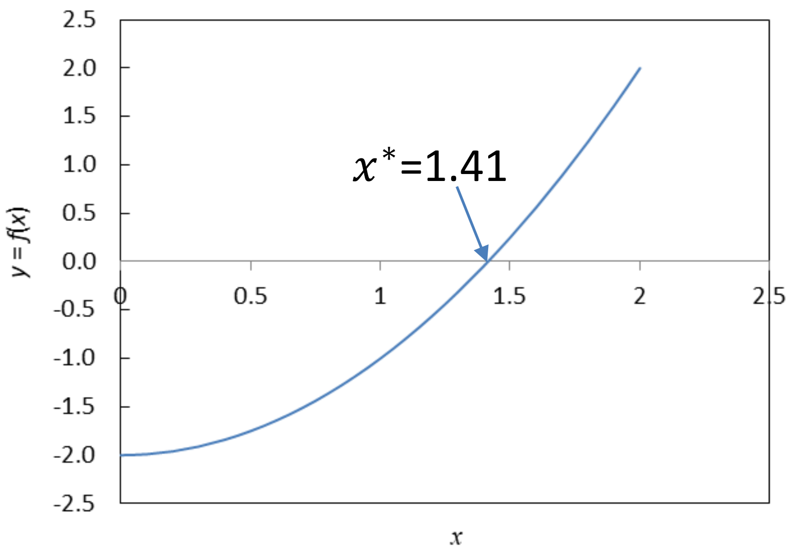
Graphical method - plot a graph between x and y=$f(x)$ and observe where the function line crosses the x –axis. That point will give as the approximate root for

Ultimately we are interested to find the value (or root) of x that satisfies $f(x) = 0$

Solution to nonlinear equation in single variable – ***Graphical method***

Iteration	*x*	*f(x)*	*f(x)*
0	0	-2.0	-2.0000
1	0.1	-2.0	-1.9900
2	0.2	-2.0	-1.9600
3	0.3	-1.9	-1.9100
4	0.4	-1.8	-1.8400
5	0.5	-1.8	-1.7500
6	0.6	-1.6	-1.6400
7	0.7	-1.5	-1.5100
8	0.8	-1.4	-1.3600
9	0.9	-1.2	-1.1900
10	1	-1.0	-1.0000
11	1.1	-0.8	-0.7900
12	1.2	-0.6	-0.5600
13	1.3	-0.3	-0.3100
14	1.4	0.0	-0.0400
15	1.5	0.3	0.2500
16	1.6	0.6	0.5600
17	1.7	0.9	0.8900
18	1.8	1.2	1.2400
19	1.9	1.6	1.6100
20	2	2.0	2.0000

$$f(x) = x^2 - 2$$



Solution to nonlinear equation in single variable – *Simple* ***Iterative method***

The *simple iterative* method used is ***successive*** approximation

- Any function in the form of

$$f(x) = 0 \qquad (1)$$

- can be transformed algebraically into the form

$$x = g(x) \qquad (2)$$

- Equations (1) and (2) are *equivalent* and therefore a *root of the equation* (2) is also root of equation (1).
- The transformation of equation (1) to (2) can be accomplished by either *algebraic manipulation* or by *adding x to both the sides* of the original equation.

Solution to nonlinear equation in single variable – *Simple* ***Iterative method***

- For example , $x^2 - 2x + 3 = 0 \Rightarrow f(x) = 0$
- Can be simply rearranged or manipulated to yield

$$\Longrightarrow x^2 + 3 = 2x$$

$$\Longrightarrow x = \frac{x^2 + 3}{2}$$

- Whereas $\sin x = 0$ could be put into the form $x = g(x)$ by adding x on both the sides to yield $x = \sin x + x$
- Thus given the *initial guess* at the root x_i equation $x = g(x)$ can be used to compute a new estimate x_{i+1} as expressed by iterative formula $x_{i+1} = g(x_i)$

Solution to nonlinear equation in single variable – *Simple* ***Iterative method***

- Therefore the approximate relative error for the iterative equation $x_{i+1} = g\,(x_i)$ is by

$$R_e = \left|\frac{x_{i+1} - x_i}{x_{i+1}}\right| \times 100$$

Solution to nonlinear equation in single variable – *Simple* ***Iterative method***

The simple iterative method used is ***successive*** approximation

- Problem : 2 Evaluate the square root of a positive number A i.e. $(\sqrt{A})$, where $A > 0$ by successive approximation method. Consider A = 2.

- Solution:
- From problem statement we have $x = \sqrt{A}$ (1)

$$(1) \Longrightarrow x = \sqrt{2} \qquad (2)$$

- The above equation (2) can be rewritten as

$$(2) \Longrightarrow x^2 = 2 \qquad (3)$$

Equation (2) can be rearranged as

$$(3) \Longrightarrow f(x) = x^2 - 2 \Longrightarrow f(x) = 0$$

$$x = g(x)$$

$$x_{i+1} = g(x_i)$$

Solution to nonlinear equation in single variable – *Simple **Iterative method***

$$(3) \Longrightarrow f(x) = x^2 - 2 \Longrightarrow f(x) = 0$$

$$x = g(x)$$

$$x^2 - 2 = 0 \qquad (4)$$

Rewrite the equation (4) as $x^2 = 2$ (5)

Add x^2 on both the sides of above equation (5) , then we have

$$x^2 + x^2 = 2 + x^2 \qquad (6)$$

Equation (6) can be simplified as

$$2x^2 = 2 + x^2 \qquad (7)$$

Divide the equation (7) by $2x$ on both the sides, and rearrange to give

$$x = \frac{2+x^2}{2x} \qquad (8)$$

The equation (8) is transformed as $x_{i+1} = \frac{2+x_i^2}{2x_i}$ which is of the form $x_{i+1} = g(x_i)$

Solution to nonlinear equation in single variable – *Simple* ***Iterative method***

i	x_i	$g(x_i)$	x_{i+1}	$R_e,\%$
0	0.5000	2.2500	2.2500	77.7778
1	2.2500	1.5694	1.5694	43.3628
2	1.5694	1.4219	1.4219	10.3773
3	1.4219	1.4142	1.4142	0.5414
4	1.4142	1.4142	1.4142	0.0015
5	**1.4142**	**1.4142**	**1.4142**	**0.0000**
6	**1.4142**	**1.4142**	**1.4142**	**0.0000**

$$g(x_i) = \frac{2 + {x_i}^2}{2x_i}$$

$$R_e = \left|\frac{x_{i+1} - x_i}{x_{i+1}}\right| \times 100$$

Solution to nonlinear equation in single variable – *Simple **Iterative method***

The simple iterative method used is ***successive*** approximation

Problem : 3 Evaluate the function $f(x) = x - \frac{1}{\sin(x)}$ by successive approximation method.

Solution:

- From problem statement we have $$x = \frac{1}{\sin(x)} \quad (1)$$

  Equation (1) can be rearranged as

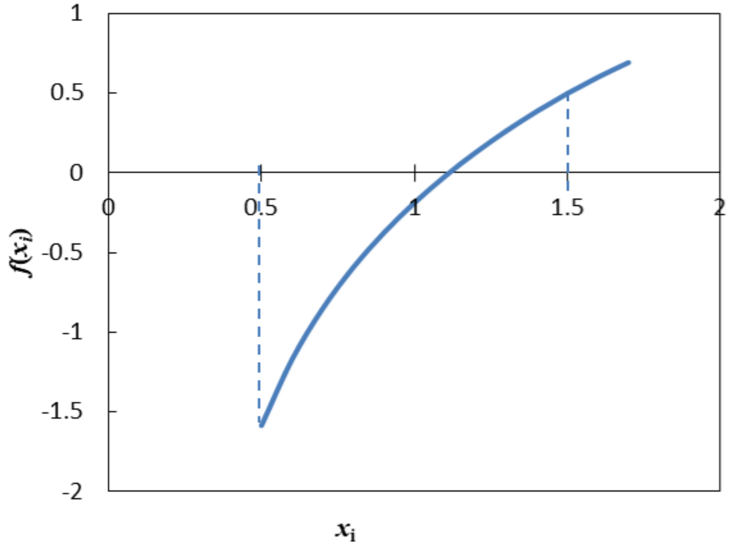
$$x = g(x)$$
$$x_{i+1} = g(x_i)$$

The initial guess may be obtained by plotting a graph between x_i and $y = f(x_i)$ and the line passing through x – axis may give an approximate root

Solution to nonlinear equation in single variable – ***Iterative method***

x_i	$f(x_i)$
0.5	-1.5858
0.6	-1.1710
0.7	-0.8523
0.8	-0.5940
0.9	-0.3766
1	-0.1884
1.1	-0.0221
1.2	0.1271
1.3	0.2622
1.4	0.3852
1.5	0.4975
1.6	0.5996
1.7	0.6916

$$f(x_i) = x_i - \frac{1}{\sin(x_i)}$$



The root may lies between 0.5 and 1.5

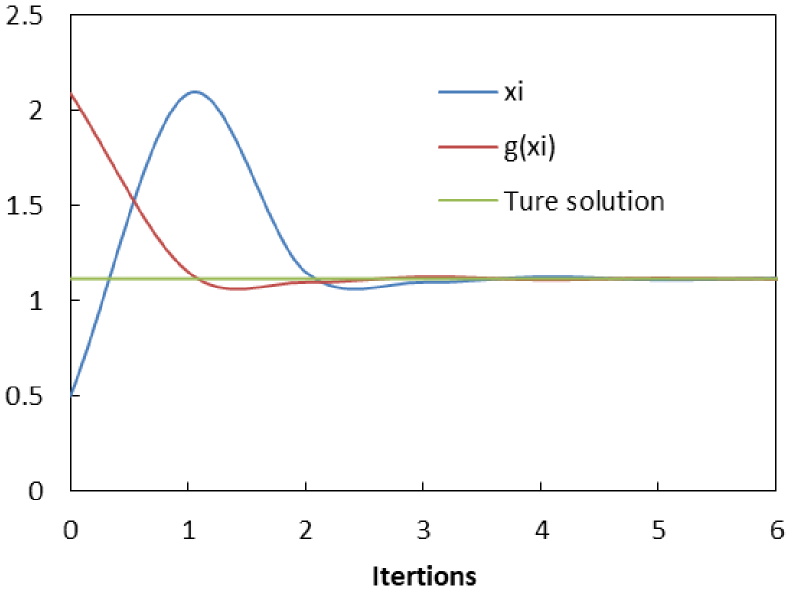
Solution to nonlinear equation in single variable – *Simple* ***Iterative method***

i	x_i	$g(x_i)$	x_{i+1}	$R_e,\%$
0	0.5	2.086	2.086	76.0
1	2.086	1.149	1.149	81.5
2	1.149	1.096	1.096	4.8
3	1.096	1.124	1.124	2.5
4	1.124	1.109	1.109	1.4
5	1.109	1.117	1.117	0.8
6	1.117	1.113	1.113	0.4
7	1.113	1.115	1.115	0.2
8	1.115	1.114	1.114	0.1
9	1.114	1.114	1.114	0.1
10	1.114	1.114	1.114	0.0
11	1.114	1.114	1.114	0.0
12	1.114	1.114	1.114	0.0

$$g(x_i) = \frac{1}{\sin(x_i)}$$

Solution to nonlinear equation in single variable – *Simple* ***Iterative method***

i	x_i	$g(x_i)$
0	0.500	2.086
1	2.086	1.149
2	1.149	1.096
3	1.096	1.124
4	1.124	1.109
5	1.109	1.117
6	1.117	1.113
7	1.113	1.115
8	1.115	1.114
9	1.114	1.114
10	1.114	1.114



Solution to nonlinear equation in single variable – *Simple* ***Iterative method***

Chemical Engineering application - Equation of State

Problem: 4 The composition of gas mixture by mole percent at 1 atm (gauge) pressure and 30°C is as follows:

N_2	= 71 %
O_2	= 19%
NH_3	= 10%

Find the weight of 100 m^3 of gas mixture using van der Waals equation of state (VDE).

Consider *a* = 135.653 x 10^{-3} Pa/(m^3/mol)^2 and *b* = 0.037 x 10-3 m^3/mol. Take, Universal Gas Constant as $R = 8.31415\ \frac{Pa\ m^3}{mol\ K}$ and pressure, $P\ i.e.1\ atm\ = 1.01325 \times 10^5$ Pa

Solution to nonlinear equation in single variable – *Simple* ***Iterative method***

Chemical Engineering application - Equation of State

Solution

$$\left(p + \frac{a}{v^2}\right)(v - b) = RT \qquad (1)$$

$$(2) \Longrightarrow \quad v = \frac{RT}{p + \frac{a}{v^2}} + b \qquad (2)$$

$$v_{i+1} = \frac{RT}{p + \frac{a}{{v_i}^2}} + b \qquad (3)$$

Solution to nonlinear equation in single variable – *Simple* ***Iterative method***

Chemical Engineering application - Equation of State

$$\rho_{mix} = \frac{1}{v} \times \sum y_i M_i \qquad (1)$$

$$(2) \Longrightarrow \quad v = \frac{RT}{p + \frac{a}{v^2}} + b \qquad (2)$$

$$v_{i+1} = \frac{RT}{p + \frac{a}{{v_i}^2}} + b \qquad (3)$$

The initial guess for equation (3) may be obtained from ideal gas equation using the relationship $PV = n\,RT \Longrightarrow \frac{V}{n} = v = \frac{RT}{P}$

Solution to nonlinear equation in single variable – *Simple **Iterative method***

Chemical Engineering application - Equation of State

The ideal gas equation can be rearranged as given below:

$$PV = n\,RT \Longrightarrow \frac{V}{n} = v_i = \frac{RT}{P}$$

$i = 0 \; in \; v_i$

$$v_o = \frac{RT}{P} = \frac{8.31415 \times 303}{1 \times 1.01325 \times 10^5}$$

$$v_o = 0.02486 \; \frac{m^3}{mol}$$

Solution to nonlinear equation in single variable – *Simple* ***Iterative method***

Now we know that $$v_{i+1} = \frac{RT}{p + \frac{a}{{v_i}^2}} + b$$

$i = 0$ in above equation then for 1st iteration we have

$$v_1 = \frac{RT}{p + \frac{a}{{v_0}^2}} + b$$

From ideal gas equation we have $v_o = 0.02486\ \frac{m^3}{mol}$ substitute this in above equation as an initial guess and iterate successively to get v_0 through Vander waal's equation. The solution is obtained and provided in next slide

Solution to nonlinear equation in single variable – *Simple* ***Iterative method***

Solution table

i	v_i	$g(v_i)$	v_{i+1}	$R_e, \%$
0	0.02486	0.02485	0.02485	0.06734
1	0.02485	0.02485	0.02485	0.00029
2	0.02485	0.02485	0.02485	0.00000
3	0.02485	0.02485	0.02485	0.00000

Solution to nonlinear equation in single variable – *Simple **Iterative method***

We know that $\rho_{mix} = \frac{1}{V} = v \times \sum y_i M_i$ (1)

Solution table for $\sum y_i M_i$ is given below

S. NO.	Components (i)	y_i	M_i	$\sum y_i M_i$
1	N_2	0.71	28	19.880
2	O_2	0.19	32	6.080
3	NH_3	0.1	17	1.700
			Total	**27.660**

Where y_i *is mole fraction of component i and* M_i *is the molecular weight of component i and it has the unit of* $\frac{kg}{mol}$ in SI

Molal volume v from Vander waal's equation through iterative procedure is obtained and it can be substituted in equation (1) to get ρ_{mix}

Solution to nonlinear equation in single variable – *Simple* ***Iterative method***

We know that $\rho_{mix} = \frac{1}{v} \times \sum y_i M_i$ where n = 1 mole

$$\rho_{mix} = \frac{1}{v} \times \sum y_i M_i = 0.02486\ \frac{\cancel{mol}}{m^3} \times 27.66\ \frac{kg}{\cancel{mol}} = 0.6877\,\text{kg/m}^3$$

1 m^3 of gas weighs 0.6877 kg

$$100\ \text{m}^3 \text{ of gas} = 100 \times \frac{0.6877}{1} = 68.77\ \text{kg}$$

References

1. Raymond P. Canale and Steven C. Chapra, Numerical Methods for Engineers, McGraw-Hill Higher Education

2. Richard Felder, Elementary principles of chemical processes, John Wiley & Sons