Some Applications of Cubic Equations in Engineering

by Jelita -

Some Applications of Cubic Equations in Engineering: Basic Theory

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Abstract

Cubic equations have many applications in engineering, three of them are discussed in this paper. There are many equations of states for real gases but the cubic equations are the simplest ones and are sufficiently accurate for a limited range of temperatures and pressures. Degree of dissociation of chemical equilibrium for carbon dioxide and water can be written as cubic equations. Slope of a simply supported beam loaded by a continuous load is also represented as a cubic equation. Although a cubic equation has three roots, only real roots are valid in real applications discussed in this paper. Even there may be only one root that can be used; two other roots will be discarded. There are many ways a cubic equation solved but the simplest one is to solve it manually using a scientific calculator. Software and programming languages are better if there are many equations to be solved repeatedly.

1. Introduction

A cubic equation is a polynomial of degree three which is generally written as

$$ax^3 + bx^2 + cx + d = 0 \tag{1}$$

where a, b, c and d are the coefficients of the equation and a is strictly not equal to zero. We are only interested for real values of the coefficients.

According to the fundamental theorem of algebra, a polynomial of degree n has n roots, including multiplicities; see [15], for example. In general, roots of a polynomial can only be found exactly for degree less than five. This theory was proved by Galois, a young French mathematician in 1830, and described in most textbooks on abstract algebra; see [5], [7] and [8], for example. Clearly, a cubic equation will have three roots, which can be divided as follow:

1. Three real roots
2. Multiple roots
3. One real root and two imaginary ones.

In engineering applications, we are usually interested in real roots only. Often we only need one real root, which must be chosen from the real roots. There are many applications of cubic equations in engineering but in this paper we will only discuss three of them.

2. Equation of State

An equation of state is an equation which relates pressure (P), temperature (T) and specific volume of a substance (v) [1], [2], [12] and [18]. Only two of those parameters are independent. Usually P and T are independent. However, most equations of state are implicit in specific volume, makes it as the independent variable together with temperature.

There are hundreds of equations of states that have been developed; [1] lists 25 of them. However, only a few of them which still remain popular. We will discuss the cubic equations of state. Cubic equations are very simple and may not represent the state of a substance very accurately except in a limited range of temperature and pressure. However, they are still useful since their simplicity makes them attractive for analysis. There are four well-known cubic equations of states i.e. the Van der Waals (VdW), Redlich-Kwong (RK), Soave (SRK), and Peng-Robinson (PR) equations. Those four equations of state will be discussed briefly. Derivations for the formulas concerned are not given; they can be found in [11].

2.1 Van der Waal's equation (Vdw)

The VdW equation is the oldest equation of state which is written as

$$P = \frac{RT}{v-b} - \frac{a}{v^2} \tag{2}$$

Eq. (2) can be arranged in terms of v as

$$v^3 - \left(b + \frac{RT}{P}\right)v^2 + \frac{a}{P}v - \frac{ab}{P} = 0 \tag{3}$$

or

$$v^3 + pv^2 + qv + r = 0 \tag{4}$$

which is a cubic equation where

$$p = -\left(b + \frac{RT}{P}\right), q = \frac{a}{P} \text{ and } r = -\frac{ab}{P} \tag{5}$$

Here, $a, b,$ and R are constants which depends on a substance.

2.2 Redlich-Kwong's equation (RK)

The RK equation is an improvement of the VdW equation and more accurate than the former. It is written as

$$P = \frac{RT}{v-b} - \frac{a}{\sqrt{T}v(v+b)} \tag{6}$$

Eq. (6) can be arranged in terms of v as

$$v^3 - \frac{RT}{P}v^2 + \left(\frac{a}{P\sqrt{T}} - \frac{bRT}{P} - b2\right)v - \frac{ab}{P\sqrt{T}} = 0 \tag{7}$$

which is similar to Eq. (4) where

$$p = -\frac{RT}{P},\ q = \frac{a}{P\sqrt{T}} - \frac{bRT}{P} - b^2,\ r = -\frac{ab}{P\sqrt{T}} \tag{8}$$

2.3 Soave equation (SRK)

Soave replaced the term $a/\sqrt{T}$ in the RK equation with a function of T and ω involving temperature and acentric factor so Eq. (6) becomes

$$P = \frac{RT}{v-b} - \frac{a\alpha}{v(v+b)} \quad (9)$$

which can be arranged in terms of v as

$$v^3 - \frac{RT}{P}v^2 + \left(\frac{a\alpha}{P} - \frac{bRT}{P} - b^2\right)v - \frac{ab\alpha}{P} = 0 \quad (10)$$

where α is given by

$$\alpha = \left[1 + (0.48 + 1.574\omega - 0.176\omega^2)\left(1 - \sqrt{T_r}\right)\right]^2 \quad (11)$$

T_r is called reduced temperature defined as T/T_c where Tc is the critical temperature while ω is the Pitzer acentric factor.

Eq. (10) is similar to Eq. (4) where

$$p = -\frac{RT}{P}, \quad q = \frac{a\alpha}{P} - \frac{bRT}{P} - b^2, \quad r = -\frac{ab\alpha}{P} \quad (12)$$

2.4 **Peng-Robinson equation (PR)**

Peng and Robinson proposed an equation of state in the form of

$$P = \frac{RT}{v-b} - \frac{a\alpha}{v^2 + 2bv - b^2} \quad (13)$$

where α is given by

$$\alpha = \left[1 + \left(0.37464 + 1.54226\,\omega - 0.26992\,\omega^2\right)\left(1 - \sqrt{T_r}\right)\right]^2 \quad (14)$$

Eq. (13) can be arranged as

$$v^3 - \left(\frac{RT}{P} - b\right)v^2 + \left(\frac{a\alpha}{P} - \frac{2bRT}{P} - 3b^2\right)v - \left(\frac{ab\alpha}{P} - \frac{b^2RT}{P} - b^3\right) = 0 \quad (15)$$

which is similar to Eq. (4) where

$$p = \frac{RT}{P} - b, \quad q = \frac{a\alpha}{P} - \frac{2bRT}{P} - 3b^2, \quad r = \frac{ab\alpha}{P} - \frac{b^2RT}{P} - b^3 \quad (16)$$

2.5 **Equations of state in terms of compressibility factor**

We can also write the equation of state of a gas as a function of compressibility factor Z. In general, a cubic equation for real gases with two parameters can be written as

$$P = \frac{RT}{v-b} - \frac{a}{v^2 + ubv + wb^2} \quad (17)$$

which is equivalent with

$$Z^3 + pZ^2 + qZ + r = 0 \quad (18)$$

where Z is the compressibility factor of the gas defined as Pv/RT. The values of p, q and r in Eq. (17) are different from those values in Eq. (4). They are given as

$$p = -(1 + B - uB), q = A + wB^2 - uB - uB^2), r = -(AB + wB^2 + wB^3) \quad (19)$$

where

$$A = \frac{aP}{R^2T^2} \quad \text{and} \quad B = \frac{bP}{RT} \tag{20}$$

In theory, there are three roots for a cubic equation. If there are three real roots found, the smallest one is taken for the saturated liquid, the biggest is for the saturated vapor while the third one is not used. If there is one real root and two imaginary ones, the real root represents the gas state while the imaginary roots are discarded.

3. Chemical Equilibrium of water and carbon dioxide

At high temperatures, gases tend to dissociate or decompose [2], [12] and [18]. Examples of dissociation reactions are as follow:

$H_2O \leftrightarrow H_2 + ½O_2$

$H_2O + O_2 \leftrightarrow 2OH$

$CO_2 \leftrightarrow CO + ½O_2$

$N_2 + O_2 \leftrightarrow NO_2$

In general, for chemical equilibrium

$$\text{aA + bB cC + dD} \tag{21}$$

where equilibrium constant K_p is defined as [2], [12] and [18].

$$K_p = \frac{P_C^c P_D^d}{P_A^a P_B^b}\left(\frac{P}{P_0}\right)^{c+d-a-b} \tag{22}$$

where P_A, P_B, P_C, and P_D are partial pressures of components in the reaction while P and P_0 are total pressure and reference pressure (which is usually atmospheric pressure), respectively. Equation (21) can also be written as

$$K_p = \frac{n_C^c}{n_A^a}\frac{n_D^d}{n_B^b}\left(\frac{P}{P_0}\frac{1}{n_t}\right)^{c+d-a-b} = \frac{[C]^c}{[A]^a}\frac{[D]^d}{[B]^b}\left(\frac{P}{P_0}\frac{1}{n_t}\right)^{c+d-a-b} \tag{23}$$

where the square bracket denotes the amount of a gas.

For the dissociation of CO_2, we have: a = 1, b = 0, c = 1 and d = 1/2. So,

$$K_p = \frac{[CO][O_2]^{1/2}}{[CO_2]}\left(\frac{P}{P_0}\frac{1}{n_t}\right)^{1/2} \tag{24}$$

We will now determine the composition of gases from the dissociation of CO_2 at temperature T and pressure P:

$CO_2 \leftrightarrow CO + ½O_2$

Let there be one mole of CO_2. After the equilibrium is achieved, CO_2 will dissociate to α mole of CO and ½α mole of O_2. The remaining amount of CO_2 is (1−α) mole. The total amount of gases is (1+½α) mole. Substituting these values to Eq. (24) results in

$$K(\alpha) = \frac{\alpha}{1-\alpha}\sqrt{\frac{P}{P_0}\frac{\alpha}{2+\alpha}} \tag{25}$$

If we denote equilibrium constant at a certain temperature T is K*, we then have

$$K^* = \frac{\alpha}{1-\alpha}\sqrt{\frac{P}{P_0}\frac{\alpha}{2+\alpha}} \quad (26)$$

The value of K* only depends on temperature, not on pressure. Most engineering thermodynamics have tables for values of equilibrium of various chemical reactions; for example, see [2] and [18].

We can remove the square root by squaring both sides in Eq. (26)

$$K^{*2} = \left(\frac{\alpha}{1-\alpha}\right)^2 \sqrt{\frac{P}{P_0}\frac{\alpha}{2+\alpha}} \quad (27)$$

By taking f = $P/(P_0K^{*2})$ and rearranging Eq. (27), we then have

$$(1-f)\alpha^3 - 3\alpha + 2 = 0 \quad (28)$$

If f ≠ 1, we can divide all terms in Eq. (28) by (1−f). We then have a depressed cubic equation where the coefficient of the second term is zero,

$$\alpha^3 + p\alpha + q = 0 \quad (29)$$

where $p = -\frac{3}{1-f}$ and $q = \frac{2}{1-f}$. If $f = 1$, the cubic term in Eq. (28) vanishes. The solution is very simple: $\alpha = \frac{2}{3}$.

It must be noted that in actual situation, there may be more than one equation that must be solved. In the given example, O_2 will also dissociate into oxygen atom. We will then have two nonlinear equilibrium reactions which are more difficult to solve. This case will not be discussed in this paper; interested readers can see [10].

4. Simply supported beam loaded by continuous load

Fig. 1 shows a beam supported at the ends and loaded by a continuous or distributed load.

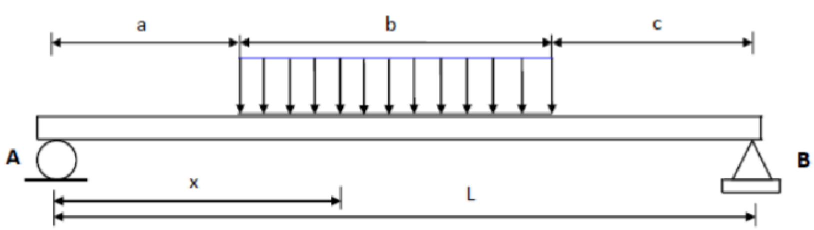

Figure 1 Simply supported beam loaded by continuous load

The deflection curve is given by the Euler-Bernoulli equation which relates the deflection with bending moment (M_x), modulus of elasticity E and moment of inertia of the cross section of the beam (I); see most textbooks on strength of materials. Most textbooks take the deflection upward as positive downward as negative; see [4], [6], [9] and [16] for example. [6] adopts the opposite ones because most deflections in engineering are downward. We will take the deflection upward as positive so the Bernoulli equation becomes

$$EI\frac{d^2Y}{dx^2} = -M_x \tag{30}$$

Integrating Eq. (30) will yield the deflection curve along the beam.

Figure 1 shows three regions where the bending moment can be applied: from 0 to a, from a to a+b and from a+b to L. Since there are three regions, there will be also three equations required for the bending moment along the length of the beam. However, we can use only one equation by adopting using singularity functions; see [16] for example.

Without derivation, the equation for the bending moment along the beam for 0 ≤ x ≤ L is given by

$$M_x = R_A x - \frac{q}{2}\langle x-a\rangle^2 + \frac{q}{2}\langle x-a-b\rangle^2 \tag{31}$$

The value <x−a> becomes zero if x−a<0 but is equal to x−a if x>a. Likewise, <x−a−b> becomes zero if x−a−b<0 but is equal to x−a−b if x>a+b. From Eq. (30) we then have,

$$EI\frac{d^2Y}{dx^2} = -R_A x + \frac{q}{2}\{\langle x-a\rangle^2 - \langle x-a-b\rangle^2\} \tag{32}$$

Integrating Eq. (32) twice produces

$$EI\frac{dY}{dx} = -R_A\frac{x^2}{2} + \frac{q}{6}\{\langle x-a\rangle^3 - \langle x-a-b\rangle^3\} + C_1 \tag{33}$$

$$EIY = -R_A\frac{x^3}{6} + \frac{q}{24}\{\langle x-a\rangle^4 - \langle x-a-b\rangle^4\} + C_1 x + C_2 \tag{34}$$

C_1 and C_2 are boundary conditions. At the supports, deflections are zero. So we then have

$X_x = 0$, $Y_A = 0 \rightarrow C1 = 0$

$X_x = L$, $Y_D = 0$, which yields

$$C_1 = R_A\frac{L^2}{6} - \frac{q}{24L}[(L-a)^4 - (L-a-b)^4] \tag{35}$$

RA can be found from the conditions that at the supports, bending moments are equal to zero. We then have

$$R_A = \frac{q}{2}[(L-a)^2 - (L-a-b)^2] \tag{36}$$

$$EIY' = \frac{q[x-a]^3}{6} - \frac{qb^2x^2}{4L} + \frac{qb^2(2L^2-b^2)}{24L} \tag{37}$$

Derivations of all formulas in this part can be done by using formulas found in most mechanics of materials (or strength of materials) textbooks such as [4], [6] and [16]. Complete formulas for various kinds of loads are given by [17].

The term inside the square bracket is zero for x ≤ a. Substituting a = L−b and arranging the terms yields

$$EIY' = \frac{q}{24L}\left\{4L[x-L+b]^3 - 6b^2x^2 + b^2(2L^2-b^2)\right\} \tag{38}$$

Now, we substitute b = mL and x = pL where 0 < m ≤ 1 and 0 ≤ p ≤ 1 to Eq. (38). After simplification and arranging the terms we then have

$$Y' = \frac{qL^3}{24EI}\left\{4[p-1+m]^3 - 6m^2p^2 + m^2(2-m^2)\right\} \tag{39}$$

Terms inside the curly brackets are dimensionless. Eq. (39) can be written as

$$Y' = f_1 f(p) \tag{40}$$

where

$$f_1 = qL^3/24EI \text{ and } f(p) = 4[p-1+m]^3 - 6m^2p^2 + m^2(2-m^2) \tag{41}$$

The equation for the deflection along the length of the beam for $0 \le x \le L$ is given by

$$EIY = \frac{q[x-a]^4}{6} - \frac{qb^2x^3}{12L} + \frac{qb^2x(2L^2-b^2)}{24L} \tag{42}$$

Substituting b = mL and x = pL to Eq. (42) results in

$$EIY = \frac{q}{24L}\left\{L[x-L+b]^4 - 2b^2x^3 + b^2x(2L^2-b^2)\right\} \tag{43}$$

which can be transformed to

$$Y = \frac{qL^4}{24EI}\left\{[p-1+m]^4 - 2m^2p^3 + m^2p(2-m^2)\right\} \tag{44}$$

Again, Terms inside the curly brackets are dimensionless. Eq. (44) can be written as

$$Y = f_2 g(p) \tag{45}$$

where

$$f_2 = qL^4/24EI \text{ and } g(p) = [p-1+m]^4 - 2m^2p^3 + m^2(2-m^2)p \tag{46}$$

The maximum deflection along the beam can be found by setting Eq. (38) to zero, which is similar to set f(p) in Eq. (39) to zero. Since f(p) is cubic, it has three roots. However, we are only interested in a real root which lies between $1-m$ and 1, which is equivalent to $a < x < L$.

5. Solving cubic equations

A cubic equation $ax^3 + bx^2 + cx + d = 0$ can be solved manually using a scientific calculator such as Casio fx-991 ES. This calculator can solve a cubic equation easily. The user just inputs the coefficients of the equation. The answer will then be displayed on the screen. The use of a calculator is very advantageous for the students who need to solve a cubic equation quickly in their study. However, for repeated uses such as in simulation the use of the calculator is very awkward and time consuming.

A cubic equation can also be solved using Excel, a very good spreadsheet. Maple, Mathematica, Mathcad or other software can also be used. We can also write a C program to solve it. Software and programming languages are better if there are many equations to be solved repeatedly. We can use exact formulas for solving the equation or solve it numerically. Usually we use Newton-Raphson method to find the roots; see [13], for example. However, it is not often easy to find the guess value for the method. At high temperature, α approaches 1; this makes Eq. (28) difficult to solve numerically. Slight change of the initial value makes the equation unstable. Various important equilibrium reactions have been analyzed by [10] not only for one equilibrium reaction but also for two and four equilibrium reactions.

While we can resort to numerical methods to solve a cubic equation, we can also find its exact roots using Cardano's or Tartaglia's formula; see [3] for an interesting discussion about the dispute on who first discovered the formula. For solving equilibrium reactions, it is better to find the exact root because it is difficult to guess the initial value as demanded by the Newton-Raphson method. For equations of state or simply supported beam problem shown in Figure 1, initial values can be easily found. A C program to solve the three problems discussed in this paper will be given in another paper

6. Conclusion

Three applications of cubic equations in engineering have been discussed. Only real roots are valid even though there are three roots in the equations. Often only one real root is used; the other two are discarded. While Newton-Raphson method is usually used to solve a cubic equation numerically, it is not easy to determine initial value for dissociation reaction that is Eq. (28). At high temperature, α approaches 1. Slight change of the initial value makes the equation unstable There are various ways for solving equation, from using a scientific calculator to programming languages. Which one used depends on the need of solving the equation.

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