A SHORT REMARK ON THE SOLUTION OF RACHFORD-RICE EQUATION

by

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A fast flash calculation of the Rachford-Rice equation is very much needed in many engineering applications, especially in multi-component mixtures. This paper suggests a direct and hands-on calculation by a pocket calculator or a Chinese abacus. The calculation is based on an ancient Chinese mathematics called as He Chengtian average. An example is given to show the simplicity and effectiveness of the ancient Chinese algorithm.

Key words: *Rachford-Rice equation, ancient Chinese mathematics, flash evaporation*

Introduction

The equilibrium flash of a multi-component liquid may be visualized as a simple distillation process using a single equilibrium stage. It is very different and more complex than the flash evaporation of single-component liquid. For a multi-component liquid, calculating the amounts of flashed vapor and residual liquid in equilibrium with each other at a given temperature and pressure requires a trial-and-error iterative solution. Such a calculation is commonly referred to as an equilibrium flash calculation. It involves solving the Rachford-Rice equation [1-4].

Flash evaporation appears in many modern technologies, such as bubble electrospinning [5, 6], and in many important equilibrium-staged separation processes [1-4, 7]. Flash calculation is essential for optimal design of the previous processes, and a fast and easy calculation is very much needed in practical applications. For a multi-component liquid, for example, a ternary solvent system in the bubble electrospinning, we use the Rachford-Rice equation [1-4, 7] to calculate the amounts of flashed vapor and residual liquid in equilibrium at a given temperature and pressure:

$$f(\psi)=\sum_{i=1}^{n}\frac{z_i(1-K_i)}{1+\psi(K_i-1)}=0 \tag{1}$$

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where z_i is the mole fraction of component i in the feed liquid, ψ – the fraction of feed that is vaporized, and K_i – the equilibrium constant of component i.

There are many theoretical methods to solve eq. (1), for example, Adomian decomposition method [7], Newton iteration method [1], and many others [2-4]. In this paper, we will suggest a hands-on calculation using an ancient Chinese mathematics.

He Chengtian inequality

He Chengtian (何承天, 369–447 AD) is a famous ancient Chinese mathematician, a brief introduction to He Chengtian inequality and its applications are referred in [8, 9].

We assume that ψ can be expressed in a simple fraction:

$$\psi = \frac{a}{b} \tag{2}$$

where a and b are positive natural numbers.

For eq. (1), it is easy to find the domain of ψ:

$$\frac{a_1}{b_1} < \psi < \frac{a_2}{b_2} \tag{3}$$

where a_1, a_2, b_1, and b_2 are known positive numbers.

A modification of He Chengtian's average of a_1/b_1 and a_2/b_2 is:

$$\psi(m,n,\lambda) = \left[\frac{m(a_1)^\lambda + n(a_2)^\lambda}{m(b_1)^\lambda + n(b_2)^\lambda}\right]^{1/\lambda} \tag{4}$$

where m, n and λ are positive numbers. For example:

$$\frac{157}{50} < \pi < \frac{22}{7}$$

The value of 22/7 has higher accurate than 157/50, so we should choose $n > m$. If we choose $m = 1$, $n = 9$, and $\lambda = 1$ we have:

$$\pi = \frac{157 + 9\times 22}{50 + 9\times 7} = \frac{355}{113}$$

This approximation improves much.

As an illustrating example, we use the data given in [7]:

$$f(\psi) = \frac{0.1(1-4.2)}{1+\psi(4.2-1)} + \frac{0.2(1-1.75)}{1+\psi(1.75-1)} + \frac{0.3(1-0.74)}{1+\psi(0.74-1)} + \frac{0.4(1-0.34)}{1+\psi(0.34-1)} =$$

$$= \frac{-0.32}{1+3.2\psi} + \frac{-0.15}{1+0.75\psi} + \frac{0.078}{1-0.26\psi} + \frac{0.264}{1-0.66\psi} = 0 \tag{5}$$

Step 1. An initial guess of the solution domain:

$$0 < \psi < 1 \tag{6}$$

Step 2. Choosing some fractals, *i. e.*, 1/2, 1/4, 1/8, 3/(24+1), …, for ψ, by direct calculation, we find:

$$f\left(\frac{3}{25}\right) = -0.0016093676 < 0 \tag{7}$$

and

$$f\left(\frac{1}{8}\right) = 0.0026442889 > 0 \tag{8}$$

It is easy to see that:

$$\frac{3}{25} < \psi < \frac{1}{8} \tag{9}$$

Step 3. Calculation of He Chengtian average:

$$\psi(1,1,2) = \sqrt{\frac{3^2+1^2}{25^2+8^2}} = \sqrt{\frac{10}{689}} = 0.120473 \tag{10}$$

The exact solution is $\psi_{\text{exact}} = 0.12188885$, while the first iteration leads to an accuracy of 1.16%. This accuracy is not better than that given in [10], but the process can continue until a needed accuracy is reached, eq. (9) can be updated:

$$\frac{4}{33} < \psi < \frac{1}{8} \tag{10}$$

Its He Chengtian average reads:

$$\psi(1,1,1) = \frac{4+1}{33+8} = \frac{5}{41} = 0.12195 \tag{11}$$

Now the accuracy is as high as 0.05%.

Conclusion

This paper suggests a simple but effective approach to flash calculations of multicomponent mixtures by He Chengtian average. The solution process can be easily carried out by a pocket calculator or a Chinese abacus. Only few iterations lead to a high accurate solution. The flash calculation is of great importance in optimal design of equilibrium-staged separation processes, and in controlling fiber size and porosity in the bubble electrospinning using multi-solvents.

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