Maximum of Ideal Mixing Entropy

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1 Weighted Arithmetic Mean and Geometric Mean Inequality

The weighted arithmetic mean and geometric mean inequality is given in the following theorem [1].

Theorem *Let the sum of the positive numbers w_i $(i = 1, 2, \cdots, n)$ be equal to 1. Then for arbitrary positive numbers a_i $(i = 1, 2, \cdots, n)$ we have the inequality*

$$w_1 a_1 + w_2 a_2 + \cdots + w_n a_n \geq a_1^{w_1} a_2^{w_2} \cdots a_n^{w_n} \tag{1}$$

with equality if and only if $a_1 = a_2 = \cdots = a_n$.

Set $b_i = \dfrac{1}{a_i}$ $(i = 1, 2, \cdots, n)$, Eq.(1) becomes

$$\frac{w_1}{b_1} + \frac{w_2}{b_2} + \cdots + \frac{w_n}{b_n} \geq \left(\frac{1}{b_1}\right)^{w_1} \left(\frac{1}{b_2}\right)^{w_2} \cdots \left(\frac{1}{b_n}\right)^{w_n} \tag{2}$$

Set

$$w_i = \frac{b_i}{b_1 + b_2 + \cdots + b_n} \qquad (i = 1, 2, \cdots, n) \tag{3}$$

we have

$$\frac{w_1}{b_1} = \frac{w_2}{b_2} = \cdots = \frac{w_n}{b_n} = \frac{1}{b_1 + b_2 + \cdots + b_n} \tag{4}$$

Substituting Eqs.(3) and (4) into Eq.(2), we obtain

$$\frac{n}{b_1 + b_2 + \cdots + b_n} \geq \left(\frac{1}{b_1}\right)^{\frac{b_1}{b_1+b_2+\cdots+b_n}} \left(\frac{1}{b_2}\right)^{\frac{b_2}{b_1+b_2+\cdots+b_n}} \cdots \left(\frac{1}{b_n}\right)^{\frac{b_n}{b_1+b_2+\cdots+b_n}} \tag{5}$$

Switch both sides and raise both sides to the power $b_1 + b_2 + \cdots + b_n$, we have

$$\left(\frac{1}{b_1}\right)^{b_1} \left(\frac{1}{b_2}\right)^{b_2} \cdots \left(\frac{1}{b_n}\right)^{b_n} \leq \left(\frac{n}{b_1 + b_2 + \cdots + b_n}\right)^{b_1+b_2+\cdots+b_n} \tag{6}$$

We write the opposite inequality for the reciprocals for above inequality,

$$b_1^{b_1} b_2^{b_2} \cdots b_n^{b_n} \geq \left(\frac{b_1 + b_2 + \cdots + b_n}{n} \right)^{b_1 + b_2 + \cdots + b_n} \tag{7}$$

and the equality holds if and only if $b_1 = b_2 = \cdots = b_n$.

2 Ideal Mixing Entropy

For an n-component solution phase, its ideal mixing entropy is

$$S = -R \sum_{i=1}^{n} x_i \ln x_i \tag{8}$$

To find the maximum of S, we write above equation as

$$S = -R \sum_{i=1}^{n} \ln x_i^{x_i} = -R \ln \prod_{i=1}^{n} x_i^{x_i} \tag{9}$$

The mole fractions, x_i ($i = 1, 2, \cdots, n$), are positive numbers. After replacing b_i in Eq.(7) by x_i, we have

$$x_1^{x_1} x_2^{x_2} \cdots x_n^{x_n} \geq \left(\frac{x_1 + x_2 + \cdots + x_n}{n} \right)^{x_1 + x_2 + \cdots + x_n} \tag{10}$$

Since $x_1 + x_2 + \cdots + x_n = 1$, Eq.(10) becomes

$$x_1^{x_1} x_2^{x_2} \cdots x_n^{x_n} \geq \frac{1}{n} \tag{11}$$

and the equality satisfies when if and only if $x_1 = x_2 = \cdots = x_n = \dfrac{1}{n}$. Combination of Eq.(9) and Eq.(11) gives

$$S = -R \ln \prod_{i=1}^{n} x_i^{x_i} \leq -R \ln \frac{1}{n} \tag{12}$$

or

$$S \leq R \ln n. \tag{13}$$

Therefore, the maximum of ideal mixing entropy is reached when $x_1 = x_2 = \cdots = x_n = \dfrac{1}{n}$ and its maximum value is $R \ln n$.

Reference

[1] Jiri Herman, Radan Kucera, Jaromir Simsa," *Equations and Inequalities: Elementary Problems and Theorems in Algebra and Number Theory*, translated by K. Dilcher, Springer, 2000.