Notes on

System Property Model

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Molar Volume and Density of a Mixture

In a thermodynamic system, we usually define a property for each phase. For a property in a multi-phase mixture system, the property of this mixture is the weighted average of the property in each phase. This weighted average is called the mean of the property mathematically.

There are many different ways to calculate the mean value. The most common mean is the arithmetic mean. Here we take molar volume and density as examples to demonstrate how to calculate a property of mixture from the properties of phases.

The molar volume (V) of a mixture of α and β phases is the weighted average of the molar volumes in α and β phases (V^α and V^β) with their molar fractions (f^α and f^β) as the weights,

$$V = f^\alpha V^\alpha + f^\beta V^\beta \tag{1}$$

Now let's see how to calculate the density of the mixture. The density (ρ) is defined as

$$\rho = \frac{M}{V} \tag{2}$$

where M is the molar mass of the mixture. The molar mass of the mixture can be calculated by

$$M = f^\alpha M^\alpha + f^\beta M^\beta \tag{3}$$

where M^α and M^β are the molar masses of the α and β phases, respectively. Substituting Eq.(1) and Eq.(3) into Eq.(2), we have

$$\rho = \frac{f^\alpha M^\alpha + f^\beta M^\beta}{f^\alpha V^\alpha + f^\beta V^\beta} \tag{4}$$

If assume that

$$M^\alpha = M^\beta = M \tag{5}$$

Eq.(4) becomes

$$\begin{aligned}\rho &= \frac{f^\alpha M + f^\beta M}{f^\alpha V^\alpha + f^\beta V^\beta} \\ &= \frac{M}{f^\alpha V^\alpha + f^\beta V^\beta} \\ &= \frac{1}{f^\alpha \frac{V^\alpha}{M} + f^\beta \frac{V^\beta}{M}} \\ &= \frac{1}{f^\alpha \frac{V^\alpha}{M^\alpha} + f^\beta \frac{V^\beta}{M^\beta}}\end{aligned} \tag{6}$$

If we define the densities of α and β phases, ρ^α and ρ^β, as

$$\rho^\alpha = \frac{M^\alpha}{V^\alpha} \tag{7}$$

$$\rho^\beta = \frac{M^\beta}{V^\beta} \tag{8}$$

the density of the mixture is expressed as

$$\rho = \frac{1}{\frac{f^\alpha}{\rho^\alpha} + \frac{f^\beta}{\rho^\beta}} \tag{9}$$

This expression says that if the molar masses of the phases in the mixture are same, the density of the mixture is the weighted harmonic mean of the densities of the phases.

Generalized Mean

This section refers to "Generalized Mean" in Wikipedia.

Assume that Z is a property of a system and z_i are the properties for the phases i $(i = 1, 2, \cdots, \phi)$. Here we use subscript to represent the phase index and the total number of phases is ϕ. If p is a real number, then the generalized mean with exponent p is

$$Z^{(p)}(z_1, z_2, \cdots, z_\phi) = (\sum_{i=1}^{\phi} f_i z_i^p)^{\frac{1}{p}} \tag{10}$$

where f_i is the molar fraction of phase i $(i = 1, 2, \cdots, \phi)$. When exponent p takes different values, we have different kinds of means of the property.

$$Z^{(-\infty)}(z_1, z_2, \cdots, z_\phi) = \min(z_1, z_2, \cdots, z_\phi) \qquad \text{minimum} \tag{11}$$

$$Z^{(-1)}(z_1, z_2, \cdots, z_\phi) = \frac{1}{\frac{f_1}{z_1} + \frac{f_2}{z_2} + \cdots + \frac{f_\phi}{z_\phi}} \qquad \text{harmonic mean} \tag{12}$$

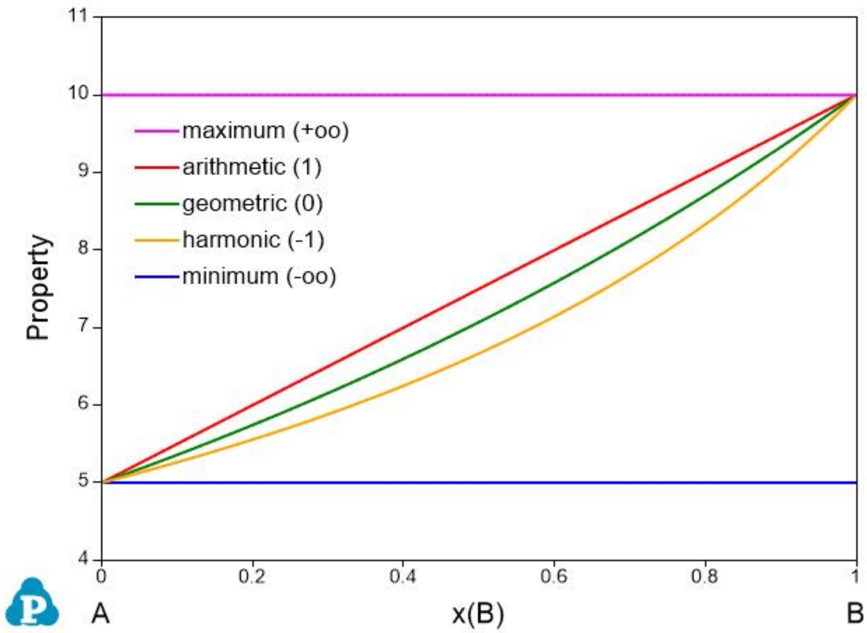
$$Z^{(0)}(z_1, z_2, \cdots, z_\phi) = {z_1}^{f_1} {z_2}^{f_2} \cdots {z_\phi}^{f_\phi} \qquad \text{geometric mean} \tag{13}$$

$$Z^{(1)}(z_1, z_2, \cdots, z_\phi) = f_1 z_1 + f_2 z_2 + \cdots + f_\phi z_\phi \qquad \text{arithmetic mean} \tag{14}$$

$$Z^{(+\infty)}(z_1, z_2, \cdots, z_\phi) = \max(z_1, z_2, \cdots, z_\phi) \qquad \text{maximum} \tag{15}$$

Example

```
Function h_A 298.15 5; 6000 N !
Function h_B 298.15 10; 6000 N !
Property minimum 298.15 min(h_A, h_B); 6000 N !
Property arithmetic 298.15 x(A) * h_A + x(B) * h_B; 6000 N !
Property harmonic 298.15 1/ (x(A) / h_A + x(B) / h_B); 6000 N !
Property geometric 298.15 exp(x(A) * ln(h_A)) * exp(x(B) * ln(h_B)); 6000 N !
Property maximum 298.15 max(h_A, h_B); 6000 N !
```



Database Format (tdb)

```
$ 1 for linear model, i.e., arithmetic mean
System_Property TCond 1 !
Parameter TCond(*;0) 298.15 ThCond_default; 3000 N !

Parameter TCond(Fcc;0) 298.15 ThCond; 3000 N !
Parameter TCond(AlCu_Theta;0) 298.15 ThCond; 3000 N !

Parameter TCond(Fcc, AlCu_Theta;0) 298.15 M0; 3000 N !
Parameter TCond(Fcc, AlCu_Theta;1) 298.15 M1; 3000 N !
Parameter TCond(Fcc, AlCu_Theta;2) 298.15 M2; 3000 N !
```