

DOI: 10.1515/amm-2016-0017

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ON THE GENERAL MATERIAL BALANCE EQUATION(S) TO CALCULATE QUASI-BINARY SECTIONS OF MULTI-COMPONENT PHASE DIAGRAMS

A general form of material balance equations to be used to calculate quasi-binary sections of multi-component phase diagrams is derived here. When this general equation is reduced to ternary systems, it coincides with those, given in the Thermo-Calc manual. For a k -component system, altogether only $(k-2)$ such independent equations should be written from the list of $k(k-1)/2$ possible equations.

Keywords: Thermo-Calc; materials balance; quasi-binary sections, multicomponent phase diagrams

Highlights

- To calculate quasi-binary sections of multicomponent phase diagrams, special materials balance equations are needed
- The general equations to calculate the numerical constants of those equations are derived here
- For a k -component system, $(k-2)$ such independent equations are needed.

1. Introduction

Ternary and multi-component phase diagrams are important tools in metallurgy and materials science [1-6]. They are usually calculated by a Calphad (Calculation of Phase Diagrams) algorithm [7-8]. Material balance equations are vital parts of this Calphad algorithm. The majority of materials balance equations are built within the commercial Calphad codes [9-15]. However, when quasi-binary sections of ternary or multi-component phase diagrams are of interest [1-6, 16-20], the user of those codes should create the appropriate materials balance equations. This is usually done in the following format (as in Thermo-Calc):

$$\alpha \cdot w_I + \beta \cdot w_J = \gamma \quad (1)$$

where I and J present two, arbitrary components in the multi-component system, w_I and w_J (dimensionless) are the mass fractions or mole fractions or volume fractions of the components, while the Greek letters denote numerical constants. The goal of this paper is to work out simple equations for numerical constants in Eq.(1), being valid for any quasi-binary section of any multi-component system.

2. Derivation of the general equations

Let us consider a multi-component system made of A - B - C -...- Z components (generally denoted as I or J). We are interested in one of its quasi-binary sections, having a horizontal concentration axis and a vertical temperature axis, with constant value of pressure. The quasi-binary section connects two alloys with each other: alloy 1 is denoted as $A_{a1}B_{b1}C_{c1}\dots Z_{z1}$, while alloy 2 is denoted as $A_{a2}B_{b2}C_{c2}\dots Z_{z2}$, where $a1, b1, c1, \dots, z1$ (generally $i1$, and $j1$) and $a2, b2, c2, \dots, z2$ (generally $i2$ and $j2$) are positive numbers defined between 0 and 1. They can be mass fractions or mole fractions or volume fractions of the components in two alloys. The materials balance requires:

$$a1 + b1 + c1 + \dots z1 = 1 \quad (2a)$$

$$a2 + b2 + c2 + \dots z2 = 1 \quad (2b)$$

It is important to underline that w_I and w_J in Eq.(1) and all parameters in Eq-s (2a-b) must have the same definition: they all should be mass fractions, or they all should be mole fractions or they all should be volume fractions.

The x -axis of the quasi-binary diagram connects alloy 1 with alloy 2, with fraction x increasing from the value equal to 0 (for alloy 1) to the value equal to 1 (for alloy 2). Then, the component fractions for two arbitrary components I and J can be written as:

$$w_I = i1 \cdot (1 - x) + i2 \cdot x \quad (3a)$$

$$w_J = j1 \cdot (1 - x) + j2 \cdot x \quad (3b)$$

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Now, let us express x from Eq.(3a) and let us substitute this equation into Eq.(3b), and finally express the result in the format of Eq.(1):

$$(j2 - j1) \cdot w_I + (i1 - i2) \cdot w_J = j2 \cdot i1 - j1 \cdot i2 \quad (4)$$

Comparing Eq.(4) with the general Eq.(1), the following expressions are found:

$$\alpha = j2 - j1 \quad (5a)$$

$$\beta = i1 - i2 \quad (5b)$$

$$\gamma = j2 \cdot i1 - i2 \cdot j1 \quad (5c)$$

Eq-s (5a-c) present the final equations of this manuscript. When applied to a ternary system, these equations simplify back to the equations provided in the ThermoCalc manual. For a quasi-binary section made of altogether k components between alloys $A_{a1}B_{b1}C_{c1}\dots Z_{z1}$ and $A_{a2}B_{b2}C_{c2}\dots Z_{z2}$, altogether $(k-1)$ materials balance equations of type (1) can be written between component A and between all other components, with the numerical coefficients to be calculated using Eq-s (5a-c). However, in fact the number of above equations can be reduced by one further equation, as Calphad codes such as ThermoCalc has the following built-in material balance equation:

$$\sum_I w_I = 1 \quad (6)$$

where $I = A, B, C, \dots, Z$.

Thus, the material balance equation for the last component may be ignored, and so for a k -component system altogether only $(k-2)$ materials balance equations of type (1) are needed. Let us note that for a k -component system altogether $k(k-1)/2$ combinations of i - j components exists. This is obviously larger than the $(k-2)$ equations needed (see Table 1). That gives the user a freedom to select arbitrary the $(k-2)$ materials balance equations, with the only condition that they should be mathematically independent. For example, for a 5-component A-B-C-D-E system in principle 10 materials balance equations of type (1) exist. However, it is sufficient to write only 3 of them, for example those, connecting components A-B, A-C and A-D. Also, in principle, equations connecting A-B, A-C and B-C could be written; however, this combination is useless, as these 3 equations are mathematically not independent.

2. Conclusions

It is shown that, to calculate quasi-binary sections of k -component phase diagrams, $(k-2)$ independent materials balance equations should be created in the format of Eq.(1). The constants in Eq.(1) are derived here and are written in Eq-s (5a-c) for any two arbitrary selected components I and J of any quasi-binary section in any multi-component system.

TABLE 1

The number of components, possible numbers of materials balance equations, their requested number to perform calculations, and their ratio

k	k(k-1)/2	(k-2)	ratio
3	3	1	3
4	6	2	3
5	10	3	3.33
6	15	4	3.75
7	21	5	4.2
8	28	6	4.67
9	36	7	5.14
10	45	8	5.63

Acknowledgements

The authors acknowledge financial support from the Hungarian Academy of Sciences, under the grant number K101781. This work is based on the results achieved within the TÁMOP-4.2.1.B-10/2/KONV-2010-0001 project and carried out as part of the TÁMOP-4.2.2.A-11/1/KONV-2012-0019 project in the framework of the New Széchenyi Plan.

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Received: 10 January 2015.

