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H. K. Abdel-Aal^a

^a CHEMICAL ENGINEERING DEPARTMENT, KING FAHD UNIVERSITY OF PETROLEUM AND MINERALS, DHAHRAN

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TECHNICAL NOTE

Use of Antoine Equation to Relate T to Y – X Equilibrium Composition

H. K. ABDEL-AAL

CHEMICAL ENGINEERING DEPARTMENT
KING FAHD UNIVERSITY OF PETROLEUM AND MINERALS
DHAHRAN 31261, SAUDI ARABIA

INTRODUCTION

The current practice followed in drawing isobaric y – x phase diagrams for a binary mixture (say Components 1 and 2) is based on data for the vapor pressure of the components as a function of temperature, T .

Calculations are initiated by first assuming a T , then finding the corresponding values for P_1 and P_2 . Equilibrium data for x and y are computed next for a given total pressure, π :

$$X_1 = \frac{\pi - P_2}{P_1 - P_2} \quad (1)$$

$$Y_1 = X_1 \frac{P_1}{\pi} \quad (2)$$

The procedure is repeated by picking different values for T .

PROPOSED RELATIONSHIP

The vapor pressure P_i of Component i is a unique property of the component and is a direct function of temperature. Thus, it increases with an increase in temperature, and a material having a higher value at a given temperature than another component is said to be *more volatile*.

Vapor pressure and temperature are commonly related by means of the well-known Antoine equation:

$$\log P_i = A_i - \frac{B_i}{C_i + T} \quad (3)$$

where A , B , and C are constants for a particular compound over a relatively narrow temperature range (up to 100°C). Values of these constants for various compounds and the applicable temperature range are given in many references (1, 2).

Now, if the values of P_1 and P_2 appearing in Eqs. (1) and (2) are replaced using the Antoine equation, the following relationships are obtained:

$$X_1 = \frac{\pi - e^{\gamma_2^{(T)}}}{e^{\gamma_1^{(T)}} - e^{\gamma_2^{(T)}}} \quad (4)$$

and

$$Y_1 = X_1 \frac{e^{\gamma_1^{(T)}}}{\pi} \quad (5)$$

where

$$\gamma_1(T) = [A_1(C_1 + T) - B_1]/(C_1 + T)$$

$$\gamma_2(T) = [A_2(C_2 + T) - B_2]/(C_2 + T)$$

Equations (4) and (5) thus establish direct relationships between T and both vapor/liquid equilibrium composition for a binary system using Antoine constants.

REFERENCES

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2. R. R. Dreisbach, "Physical Properties of Chemical Compounds I, II and III," *Am. Chem. Soc. Adv. Chem. Ser.*, 15 (1955); 29 (1961).

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