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Publisher *Taylor & Francis*

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## Separation Science and Technology

Publication details, including instructions for authors and subscription information:

<http://www.informaworld.com/smpp/title~content=t713708471>

### Use of Antoine Equation to Relate T to Y-X Equilibrium Composition

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**To cite this Article** Abdel-Aal, H. K.(1995) 'Use of Antoine Equation to Relate T to Y-X Equilibrium Composition', Separation Science and Technology, 30: 15, 3087 – 3088

**To link to this Article:** DOI: 10.1080/01496399508013131

URL: <http://dx.doi.org/10.1080/01496399508013131>

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TECHNICAL NOTE

**Use of Antoine Equation to Relate  $T$  to  $Y$ - $X$  Equilibrium Composition**

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**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,  $\pi$ :

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

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

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).

Received by editor November 30, 1994