

HIGHLY ACCURATE CORRELATING METHOD FOR PHASE EQUILIBRIUM DATA,
AND PHASE EQUILIBRIUM CALCULATION METHOD

ABSTRACT

Provided are a method for precisely predicting phase equilibrium from existing phase equilibrium data on the basis of a wide range of phase equilibrium data including binary vapor-liquid equilibrium data; a method or apparatus for designing or controlling a component separator or a refiner using the prediction method; and a program for designing this design or control apparatus.

Binary phase equilibrium measurement data is used to calculate an index X of proximity ratio to critical points that is represented by the following equation (22) and infinite dilution pressure gradients Y_1 and Y_2 that are represented by the following equations (24) and (25):

Index X of proximity ratio to critical points:

[Formula 1]

$$X = \frac{p_{1s} + p_{2s}}{P_{c1} + p_{2s}} \quad (22)$$

Infinite dilution pressure gradients Y_1 and Y_2 :

[Formula 2]

$$Y_1 = \frac{\gamma_1^\infty p_{1s} - p_{2s}}{P_{c1} - p_{2s}} \quad (24)$$

[Formula 3]

$$Y_2 = \frac{p_{1s} - \gamma_2^\infty p_{2s}}{P_{c1} - p_{2s}} \quad (25)$$

wherein P_{c1} represents the critical pressure of component 1 in the binary system; p_{1s} and p_{2s} represent the vapor pressures of components 1 and 2, respectively, at a temperature T; and γ_i^∞ represents the infinite dilution activity coefficient of component i in the liquid phase.

The obtained index X is correlated with Y_1 and Y_2 to newly calculate infinite dilution activity coefficients γ_1^∞ and γ_2^∞ or binary parameters A and B from the X - Y_1 correlation and the X - Y_2 correlation, respectively. The obtained values of γ_1^∞ and γ_2^∞ or A and B are used to predict phase equilibrium. The thus obtained values are used to design or control a component separator or a refiner, such as a distillation column.