ผลของความไม่แม่นยำของแบบจำลองสมบัติเทอร์โมไดนามิกส์ที่มีต่อการจำลองการกลั่น

นางสาววันทนา สมเจริญวัฒนา

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EFFECT OF INACCURACY OF A THERMODYNAMIC PROPERTY MODEL ON DISTILLATION SIMULATION

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วันทนา สมเจริญวัฒนา : ผลของความไม่แม่นยำของแบบจำลองสมบัติเทอร์โมไดนามิกส์ที่มีต่อการจำลองการกลั่น (EFFECT OF A THERMODYNAMIC PROPERTY MODEL ON DISTILLATION SIMULATION) อาจารย์ที่ปรึกษา : รศ.ดร.เกริกชัย สุกาญจนัจที 295 หน้า. ISBN 974-130-609-1

งานวิจัยนี้ได้ศึกษาขนาดของความผิดพลาดของผลการจำลองการกลั่นเมื่อใช้ข้อมูลสมบัติที่ไม่ถูกต้องและได้ทำการสังเกตผลโดยแยกกันของความไม่แม่นยำของแบบจำลองสมดุลไอ-ของเหลวและแบบจำลองเอนธัลปีที่มีต่อผลการจำลองการกลั่นงานวิจัยนี้ยังศึกษาเกี่ยวกับความแม่นยำของแบบจำลองสมบัติที่ใช้ด้วยโดยงานวิจัยนี้ใช้ระบบเอธานอลและน้ำในการศึกษา นอกจากนี้ยังศึกษาผลของอัตราส่วนป้อนกลับและจำนวนขั้นตอนสมดุลที่มีต่อการจำลองการกลั่นขณะที่ใช้แบบจำลองสมบัติที่ไม่ถูกต้องด้วย จากงานวิจัยนี้สามารถสรุปได้ดังนี้

1.ความผิดพลาดของค่าคงที่สมดุลนั้นจะส่งผลอย่างมากกับการจำลองการกลั่น โดยพบว่าการจำลองการกลั่นที่ใช้ค่าคงที่สมดุลที่มีความผิดพลาดเกิน±9%จะให้ผลที่ไม่สามารถยอมรับได้

2.ความผิดพลาดของเอนธัลปีจะไม่ส่งผลต่อการจำลองการกลั่นแม้ว่าความผิดพลาดจะสูงถึง±37% ผลการจำลองการกลั่นก็ยังยอมรับได้

ดังนั้นเพื่อความถูกต้องแม่นยำของผลการจำลองการกลั่นแล้วจะต้องใช้ค่าคงที่สมดุลที่ถูกต้องแม่นยำ

ภาควิชา...**วิศวกรรมเคมี**... **ลายมือชื่อนิสิต**......................................
สาขาวิชา...**วิศวกรรมเคมี**... **ลายมือชื่ออาจารย์ที่ปรึกษา**........................
ปีการศึกษา...**2543**..........

#4070413121 : MAJOR CHEMICAL ENGINEERING

KEY WORD: DISTILLATION SIMULATION / DISTILLATION / ETHANOL+WATER

WANTANA SOMCHAROENWATTANA: EFFECT OF INACCURACY OF A THERMODYNAMIC PROPERTY MODEL ON DISTILLATION SIMULATION. THESIS ADVISOR: ASSO. PROF. KROEKCHAI SUKANJANAJTEE, Ph.D. 295 pp. ISBN 974-130-609-1.

This work is to study the extent of error in distillation simulation result when inaccurate property data are used. The effect of inaccuracy in both vapor-liquid equilibrium model and enthalpy model on the distillation simulation result are investigated separately. This work also involves determining the accurate property models used. This study is based on the system ethanol+water. The effect of reflux ratio and number of equilibrium staged on distillation simulation result was also studied with inaccurate property model. From this work, it can be concluded that :

1. The error in the K-value will have great effect on distillation simulation result. Distillation simulation with error in K-value exceeding ±9% should not be acceptable.
2. The distillation simulation is not sensitive to the error in enthalpy. Even though the error is as high as ±37%, the simulation result is still acceptable.

For good simulation result, the accurate K-value must be used.

Department…of Chemical Engineering………. Student’s signature…………………………

Field of study…Chemical Engineering……….. Advisor’s signature…………………………

Academic year…2000………………………….. Co-Advisor’s signature……………………...

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CONTENTS

Page

CHAPTER

Page

Page

LIST OF TABLES

Page

Page

Page

Page

Page

Page

LIST OF FIGURES

Figure **Page**

Page

Page

CHAPTER 1

INTRODUCTION

Distillation is the most widely used separation method to be found in the chemical and petroleum industries. It is a method of separation based on the difference in composition between a liquid mixture and the vapor formed from it. The composition difference is due to differing effective vapor pressures, or volatilities, of the components of the liquid. The mixture is physically separated into two or more product in this process.

As stated above, the difference in volatility of the various components of a liquid mixture is a key to the successful application of distillation. This difference can be related to the thermodynamic equilibrium that can exist between the liquid and vapor mixtures under conditions that can be associated with the distillation at hand. The phase equilibrium relationships are embodied in general area of solution thermodynamics and can be measured or, in a same cases, predicted from the properties of pure materials involved. The resulting equilibrium compositions often are referred to as vapor-liquid equilibrium data, shortened to vapor-liquid equilibria and abbreviated simply as VLE. There are occasional instances when a second immiscible liquid phase is involved, with compositions of the three phases at thermodynamic equilibrium known simply as vapor-liquid-liquid equilibria, or VLLE.

Computer simulation of distillation has been widely used in process design and prediction of operating performance. In distillation simulation, the following property data of the mixture are needed : vapor-liquid equilibrium data, enthalpy-concentration data and fugacity. For convenience, these data are represented by thermodynamic property models or excess properties of mixtures.

Various thermodynamic property models are available. For example, vapor-liquid equilibria data (VLE) can be correlated by either Wilson equation, van Laar equation, Margules equation, or NRTL equation. Fugacity model can be derived based on a chosen equation of state (EOS) such as Virial EOS, Soave-Redlich-Kwong EOS or Peng-Robinson EOS. Enthalpy correlation requires an equation of state and ideal gas state heat capacity model.

Accuracy in reproducing experimental property data depends on property model selected. Thus, the result of distillation simulation will depend on the property model used. Distillation process design needs accuracy. This calls for an accurate property model of the system involved. However, in many cases, accurate property model is not available. Thus an engineer must use his own judgment in evaluating the simulation result. Knowledge learned from this research should be useful to him.

1.1 Objective

To study the effect of inaccuracy in thermodynamic property model on distillation simulation.

1.2 Scope

(a) Determine the accuracy of property models to be used.

(b) Determine separately, the effect of VLE model and enthalpy model on the results of distillation simulation.

(c) Study the above effect at various equilibrium of stages and reflux ratios.

(d) System used is ethanol(1) + water(2) mixture.

CHAPTER 2

DISTILLATION

Distillation is broadly defined as the separation of more volatile materials from less volatile materials by a process of vaporization and condensation. In engineering terminology, the separation of a liquid from a solid by vaporization is considered evaporation, and the term distillation is reserved for the separation of two or more liquids by vaporization and condensation.

Distillation is based on the difference in composition between a liquid mixture and the vapor formed from it .The composition difference is due to differing vapor pressures, or volatilities, of the components of the liquid. When such a difference does not exist, as at an azeotropic point, separation by distillation is not possible. The most elementary form of the method is simple distillation in which the liquid mixture is brought to boiling and the vapor formed is separated and condensed to form product; if the process is continuous, it is called flash distillation or an equilibrium flash, and if the feed mixture is available as an isolated batch of material, the process is a form of batch distillation and the compositions of the collected vapor and residual liquid are thus time dependent.

The term fractional distillation originally was applied to the collection of separations of condensed vapor, each fraction being segregated. Currently, the term is applied to distillation separations in general, where an effort is made to separate an original mixture into several components by means of distillation. When the vapors are enriched by contact with counterflowing liquid reflux, the process often is called rectification. When operated with a continuous feed of liquid mixture and continuous removal of product fractions, the process is continuous distillation, When steam is added to the vapors to reduce the partial pressures of the components to be separated, the term steam distillation is used; if such a process is altered to eliminate the steam, dry distillation (conventional distillation) results.

Most distillations conducted commercially operate continuously, with a more volatile fraction recovered as distillate and a less volatile fraction remaining as residue or bottoms, If a portion of the distillate is condensed and returned to the process to enrich the vapors, the liquid is called reflux. The apparatus in which the enrichment occurs is usually a vertical, cylindrical vessel called a still or distillation column. This apparatus normally contains internal devices for effecting vapor-liquid contact; the devices may be trays or packings.

As stated above, a separation by distillation involves differing volatilities of the components to be separated, If the volatility difference is so small that an adequate separation cannot be made, it may be possible to increase the volatility difference by the addition of an extraneous material that can be separated later; this process is known as extractive distillation if the added material is relatively nonvolatile and leaves the column with the residue. If the added material forms an azeotrope with one or more of the components of the mixture and in so doing enhances the separability of the original mixture, azeotropic distillation results. In this last-named mode, the extraneous material, or azeotropic agent, may leave the column in the distillate (low-boiling azeotrope) or in the residue (high-boiling azeotrope).

It is clear that the difference in volatility of the various components of a liquid mixture is a key to the successful application of distillation. This difference can be related to the thermodynamic equilibrium that can exist between the liquid and vapor mixtures under conditions that can be associated with the distillation at hand. The phase equilibrium relationships are embodied in general area of solution thermodynamics and can be measured or, in a same cases, predicted from the properties of pure materials involved. The resulting equilibrium compositions often are referred to as vapor-liquid equilibrium data, shortened to vapor-liquid equilibria and abbreviated simply as VLE. There are occasional instances when a second immiscible liquid phase is involved, with compositions of the three phases at thermodynamic equilibrium known simply as vapor-liquid-liquid equilibria, or VLLE.

2.1 Distillation processes

Basic distillation involves application of heat to a liquid mixture, vaporization of part of the mixture and removal of the heat from the vaporized portion. The resultant condensed liquid, the distillate, is richer in the more volatile components and the residual unvaporizes bottoms are richer in the less volatile component. Most commercial distillations involve some form of multiple staging in order to obtain a greater enrichment than is possible by a single vaporization and condensation.

Simple Distillation. Simple distillations utilize a single equilibrium stage to obtain separation. Simple distillations may be either batch or continuous. Simple batch distillation (also called differential distillation) is not widely used in industry.

Simple continuous distillation (also called flash distillation) has a continuous feed to an equilibrium stage; the liquid and vapor leaving the stage are in phase equilibrium. A schematic representation is shown in Figure 1. The feed is represented by x_L^F, the bottoms liquids by x_L^B, and the equilibrium vapor distillate by y_L^D.

The mass balance are:

$$F = D + B \qquad \text{(overall balance)} \qquad (2\text{-}1)$$

$$x_L^F F = y_L^D D + x_L^B B \qquad \text{(component balance)} \qquad (2\text{-}2)$$

Flash distillations are widely used where a crude separation is adequate.

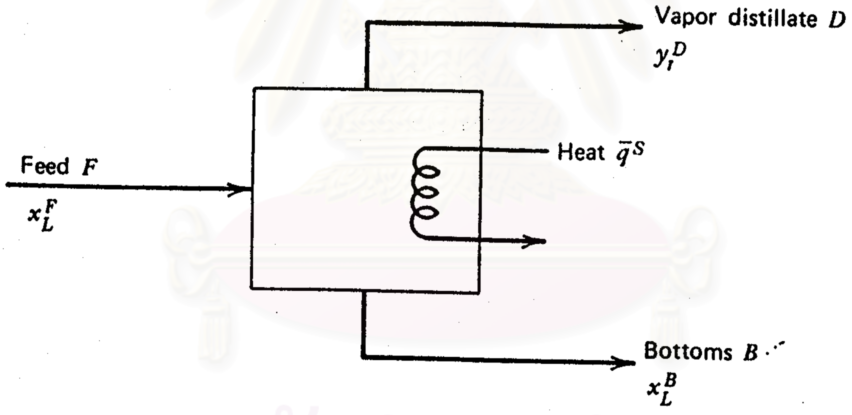


Figure2.1 Simple continuous distillation with single equilibrium stage.

Multiple Equilibrium Staging. The component separation in simple distillation is limited to the composition difference between liquid and vapor in phase equilibrium; multiple equilibrium staging is used to increase the component separation. Figure 2.1 schematically represents a continuous distillation that employs multiple equilibrium stages stacked one upon another.The feed F enters the column at equilibrium stage($\bar{f}$).

The heat ($\bar{q}^{s}$) required for vaporization is added at the base of the column in a reboiler or calandria. The vapors (V^T) from the top of the column flow to a condenser from which heat ($\bar{q}^{c}$) is removed. The liquid condensate from the condenser splits into two streams: the first, a distillate (D) which is the overhead product (also called heads or make) is withdrawn from the system and the second, a reflux (R) is returned to the top of the column. A bottoms stream (B) is withdrawn from the reboiler. The overall separation is the feed *F* separating into a distillate (D) and a bottoms (B).

Above the feed a typical equilibrium stage is designated as n; the stage above n is n+1 and the stage below n is n-1. The section of column above the feed is called the rectification section and the section below the feed is referred to as the stripping section. The mass balance across stage n is : (1) Vapor (V^{n-1}) from the stage below(n-1) flows up to stage n; (2) The liquid (L^{n+1}) from the stage above (n+1) flows down to stage n; (3) On stage (n) the vapors leaving (V^{n})are in equilibrium with the liquid leaving (L^{n}). The vapors moving up the column from equilibrium stage to equilibrium stage are increasingly enriched in the more volatile components. Similarly, the liquid streams moving down the column are increasingly diminished in the more volatile components. The overall column mass balances are:

$$F = D + B \qquad (2\text{-}3)$$

And for any component i :

$$Fx_i^F = Dx_i^D + Bx_i^B \qquad (2\text{-}4)$$

A mass balance around plate n and the top of the column gives:

$$V^{n-1} = L^{n} + D \qquad (2\text{-}5)$$

And for any component:

$$V^{n-1}y_i^{n-1} = L^{n}x_i^{n} + Dx_i^D \qquad (2\text{-}6)$$

$$\therefore y_i^{n-1} = \left(\frac{L^n}{V^{n-1}}\right)x_i^n + \left(\frac{D}{V^{n-1}}\right)x_i^D \qquad (2\text{-}7)$$

Below the feed, a similar balance around plate m and the bottom of the column results is:

$$\therefore y_i^{m-1} = \left(\frac{L^m}{V^{m-1}}\right)x_i^m + \left(\frac{D}{V^{m-1}}\right)x_i^m \qquad (2\text{-}8)$$

Equation (2-7) is the upper (or rectifying) operating line equation and equation (2-8) the lower (or stripping) operating line equation.

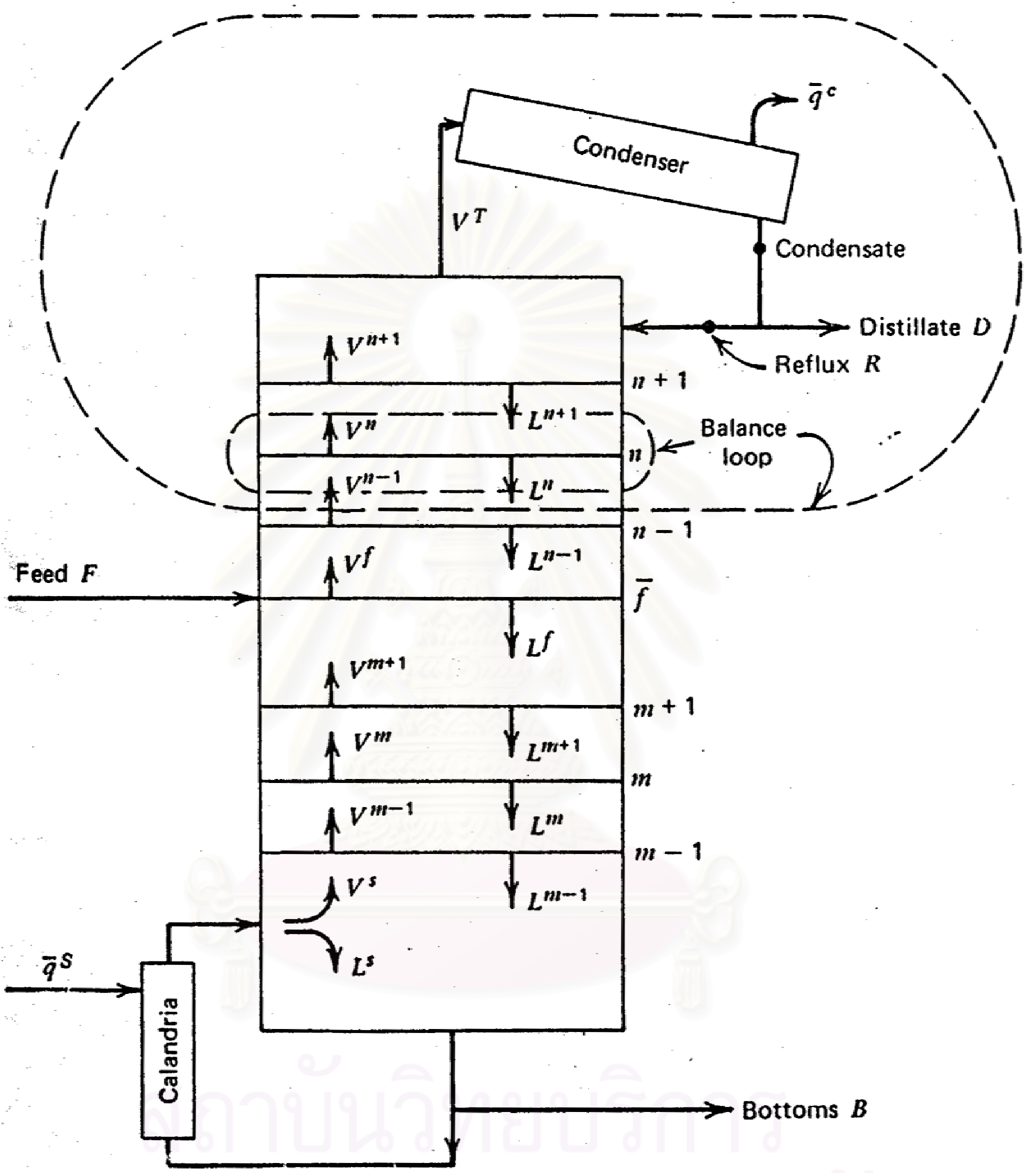


Figure2.2 Distillation column with stacked multiple equilibrium stages.

2.2 Mathematical Model for Distillation

For the convenience of deriving the general working equations, a hypothetical system as shown in Figure 2.3 is considered as the model column. This column has *n* equilibrium stages including a condenser (partial, total or compound condenser) and a reboiler. The stages (trays or plates) are numbered from top to bottom with the condenser as the first stage and the reboiler as the *n*th stage. It is assumed that one feed stream F_j, one vapor side stream W_j, one liquid side stream U_j, and one intercooler or interheater Q_j, exist at each stage except for the condenser and the reboiler. This model column can be reduced to any simpler one by setting the undesired quantified to zero. Thus for a conventional column all the quantities of the external streams except F_j, Q_D, Q_B, D, and B are zero. Each stage in the model column is assumed to be an equilibrium stage, that is, the vapor stream leaving the stage is in equilibrium with the liquid stream leaving the same stage. Figure 2.4 shows such an ideal equilibrium stage.

The MESH EQUATIONS. There are generally four sets of equations which must be satisfied in a rigorous equilibrium stage calculation. They are the material balance equation (M), the equilibrium equation (E), the summation equilibrium equation (S) of mole fractions, and the heat balance equation (H). These four sets of equations are designated as MESH equations in this article.

In this work, the material and heat balances are written around each stage and the independent variables are the mole fractions of liquid x_{ij}, the vapor rate profile V_j, and the temperature profile T_j.

Referring to Figure 2.3 and 2.4, the MESH equations for the model column are readily derived as follows:

M − Equation:

$$M_{ij}(x_{ij}, V_j, T_j) = L_{j-1}x_{i,j-1} - (V_j + W_j)y_{ij} - (L_j + U_j)x_{ij} + V_{j+1}y_{i,j+1} + F_j z_{ij} = 0 \qquad (2-9)$$

E − Equation:

$$E_j(x_{ij}, V_j, T_j) = y_{ij} - K_{ij}x_{ij} = 0 \qquad (2-10)$$

S−Equation:

$$S_j(x_{ij},V_j,T_j)=\sum_{i=1}^{m} y_{ij}-1=0 \qquad (2\text{-}11)$$

or

$$S_j(x_{ij},V_j,T_j)=\sum_{i=1}^{m} x_{ij}-1=0 \qquad (2\text{-}11a)$$

H−Equation

$$H_j(x_{ij},V_j,T_j)=L_{j-1}H_{L,j-1}-(V_j+W_j)H_{V,j}-(L_j+U_j)H_{L,j}+V_{j+1}H_{V,j+1}+F_jH_{Fj}-Q_j=0 \quad (2\text{-}12)$$

Equation (2-9) and (2-10) are now combined and the L's are expressed as function of V's by on overall material balance of all stages from the condenser through the jth tage.

$$L_j=V_{j+1}+\sum_{k=2}^{j}(F_k-W_k-U_k)-D \qquad 2\leq j\leq n\text{-}1 \qquad (2\text{-}13)$$

where $D = V_1+U_1$ (2-14)

Solution of the MESH equation

The M-equation is then reduced to a tridiagonal matrix form,

$$B_1x_{i1}+C_1x_{i2}=D_1 \qquad (2\text{-}15)$$

$$A_jx_{i,j-1}+B_jx_{ij}+C_jx_{i,j+1}=D_j \qquad 2\leq j\leq n\text{-}1 \qquad (2\text{-}16)$$

$$A_nx_{i,n-1}+B_{nj}x_{in}=D_n \qquad (2\text{-}17)$$

or in matrix notation as,

$$\begin{bmatrix} B_1 & C_1 & & & \\ A_2 & B_2 & C_2 & & \\ & A_j & B_j & C_j & \\ & & A_{n-1} & B_{n-1} & C_{n-1} \\ & & & A_n & B_n \end{bmatrix}\begin{bmatrix} x_{i1} \\ x_{i2} \\ x_{ij} \\ x_{i,n-1} \\ x_{in} \end{bmatrix}=\begin{bmatrix} D_1 \\ D_2 \\ D_j \\ D_{n\text{-}1} \\ D_n \end{bmatrix} \qquad (2\text{-}18)$$

or simply,

$$\left[A_{B_c}\right]\left\{x_{ij}\right\}=\left\{D_j\right\} \qquad 1\leq i\geq m \qquad (2\text{-}19)$$

where;

$$B_1 = -(V_1K_{i1} + U_1) \quad ; \quad C_1 = V_2K_{i2} \quad ; \quad D_1 = 0 \qquad (2\text{-}20)$$

$$A_j = L_{j-1} = V_j + \sum_{k=2}^{j-1}(F_k - W_k - U_k) - D \qquad 2 \le j \le n\text{-}1 \qquad (2\text{-}21a)$$

$$B_j = -\left[(V_j + W_j)K_{ij} + (L_j + U_j)\right]$$

$$= -\left[(V_j + W_j)K_{ij} + V_j + \sum_{k=2}^{j-1}(F_k - W_k - U_k) - D + U_j\right] \qquad 2 \le j \le n\text{ - }1 \qquad (2\text{ - }21b)$$

$$C_j = V_{j+1}K_{j+1} \qquad 2 \le j \le n\text{-}1 \qquad (2\text{-}21c)$$

and

$$A_n = V_n + B \quad ; \quad B_n = -(V_nK_{in} + B) \quad ; \quad D_n = 0 \qquad (2\text{ - }22)$$

With the above manipulation of the M and E equations and further manipulations of the S and H equations, the MESH equations for multicomponent separation at constant pressure in a complex column become,

$$M_{ij}(x_{ij}, V_j, T_j) = \left[A_{B_C}\right]\{x_i\} - \{D\} = 0 \qquad 1 \le i \le m \text{ and } 1 \le j \le n \qquad (2\text{-}23)$$

$$S_j(x_{ij}, T_j) = \sum_{i=1}^{m} K_{ij}x_{ij} - 1 = 0 \qquad 1 \le j \le n \qquad (2\text{-}24)$$

$$H_j(x_{ij}, V_j, T_j) = \left(H_{Vj+1} - H_{Lj}\right)V_{j+1} - \left(H_{Vj} - H_{Lj}\right)\left(V_j + W_j\right) - \left(H_{Lj} - H_{Lj-1}\right)L_{j+1} + F_j\left(H_{Fj} - H_{Lj}\right) - Q = 0;$$
$$1 \le j \le n \qquad (2\text{-}25)$$

There are n(m+2) independent variables in these n(m+2) equations and therefore this system of equations is consistent. The problem now is to find a set of values of x_{ij}, V_j, and T_j, to satisfy these MESH-equations. Because of their non-linear nature, a direct simultaneous solution is very difficult if not impossible. Consequently, the solution is generally obtained by using some iterative procedure is presented in the following sections.

The Tridiagonal Matrix Method

When the flow rates and compositions of feed streams are given, and the amounts of all the product streams are specified, F_j, Z_{ij}, W_j, U_j, D, and B are all constants. If an initial set of V_j and T_j is assumed, $[A_{BC}]$ and {D} are also constant, provided that the equilibrium ratios, K_{ij} 's, can be expressed as functions of T_j's. Then the M-equation, Equation (2-23), is a linear system. By taking advantage of the tridiagonal form of the matrix $[A_{BC}]$ and by grouping the vector {D} with $[A_{BC}]$as:

$$\begin{bmatrix} B_1 & C_1 & & & & D_1 \\ A_2 & B_2 & C_2 & & & D_2 \\ & A_j & B_j & C_j & & D_j \\ & & A_{n-1} & B_{n-1} & C_{n-1} & D_{n-1} \\ & & & A_n & B_n & D_n \end{bmatrix} ;1 \leq i \leq m \qquad (2\text{-}26)$$

solution of equation (2-23) for $[x_{ij}]$ can be easily obtained by use of a simple algorithm derived from the Gauss elimination method. In this algorithm, two auxiliary quantities, p_j and q_j are calculated by first evaluating p_1 and q_1 and advancing forward with j increasing, that is,

$$p_1 = C_1 / B_1 \; ; \; q_1 = D_1 / B_1 \qquad (2\text{-}27a)$$

$$p_j = C_j /(B_j - A_j p_{j-1}) \qquad 2 \leq j \leq n\text{-}1 \qquad (2\text{-}27b)$$

$$q_j = (D_j - A_j q_{j-1})/(B_j - A_j p_{j-1}) \qquad 2 \leq j \leq n\text{-}1 \qquad (2\text{-}27c)$$

Then, values of x_{ij}'s are calculated by first evaluating x_{in} and receding backward with j decreasing until x_{i1} is reached. Thus,

$$x_{in} = q_n \qquad (2\text{-}28a)$$

$$x_{ij} = q_j - p_j x_{i,j+1} \qquad 1 \leq j \leq n\text{-}1 \qquad (2\text{-}28b)$$

When the x's obtained from the above algorithm are substituted into S-equation, Equation (2-24). and if K_{ij}'s could calculate from VLE correlation (that obtained in next section) as function of T .

$K_{ij} = f(T,P, x_i, y_i)$

The S- equation is function of K_{ij} , so it is a function of T_j.

$S_j = f(T_j,...)$

The solution of this equation calculated by computer, and the process is repeated until

$S_{ik} = S_j(T_{ik}) \leq \varepsilon$

where, ε is a tolerance.

When finished the process , we will received value of T_j (temperature profile). The value of T_j is used to calculate the enthalpies(H) of streams, that is obtained in next section.

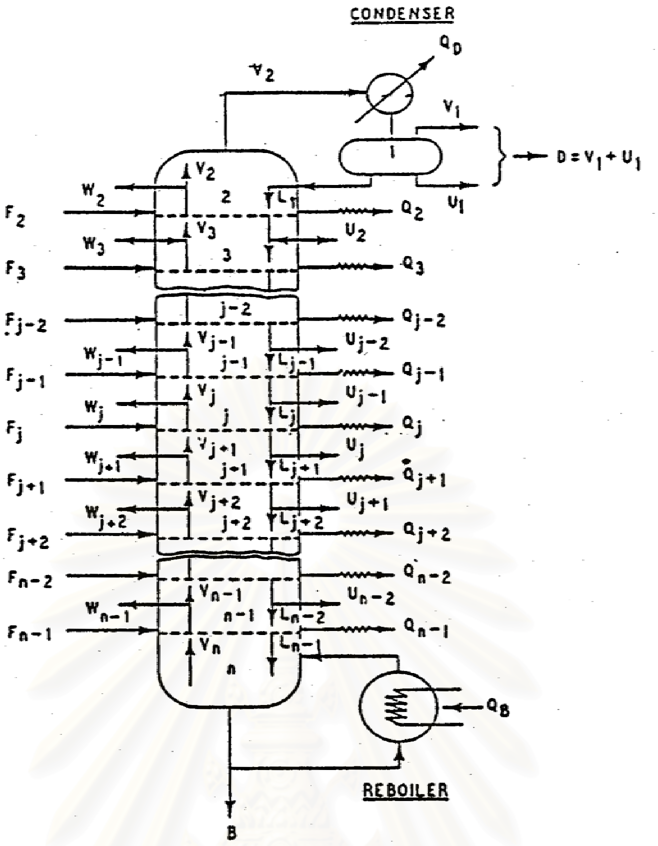


Figure2.3 A material balance is solved simultaneously for each component.

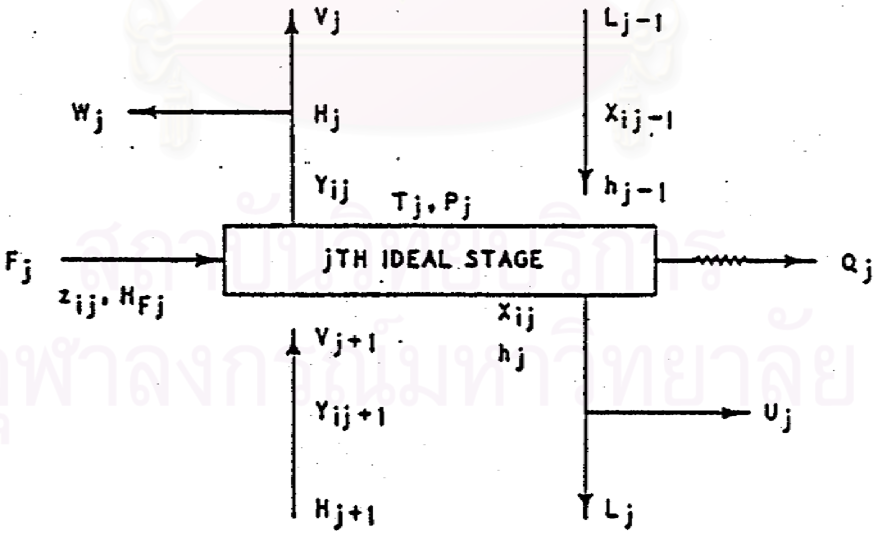


Figure2.4 An ideal equilibrium stage is represented by Equations (2-9)-(2-13).

CHAPTER 3

THERMODYNAMIC PROPERTIES

3.1 Vapor-Liquid Equilibrium (VLE)

Vapor-liquid equilibrium is the relationship of the composition of vapor phase and the liquid phase when the phases are in physical equilibrium. The driving force for any distillation is a favorable VLE; if the VLE are unfavorable, the distillation is impossible. Reliable VLE data are essential for distillation column design and for most operations involving liquid-vapor-phase contacting. VLE data come from various sources such as in-house or contract experimental measurements or the literature. If the data are not available, they may be measured or estimated. Whatever their source, some evaluation should be made regarding accuracy. The VLE for the system at hand may be simple and easily represented by an equation or, in some systems, may be so complex that they cannot be adequately measured or represented.

At equilibrium $$\hat{f}_i^{V} = \hat{f}_i^{L} \qquad (i = 1,2,...n) \qquad (3 - 1)$$

definition of fugacity coefficient of component i in solution :

$$\hat{\phi}_i \equiv \hat{f}_i / x_i P \qquad (3 - 2)$$

Thus, letting x_i , y_i represent a liquid and vapor - phase mole fractions, we can write

$$\hat{f}_i^{V} = \hat{\phi}_i y_i P \quad \text{and} \quad \hat{f}_i^{L} = \hat{\phi}_i y_i P \qquad (3 - 3)$$

The liquid - phase fugacity in equation (3 - 1) are eliminated in favor of activity coefficients, as defined by

$$\gamma_i \equiv \frac{\hat{f}_i}{x_i f_i}$$; f_i is fugacity of pure specie i in liquid phase at T, P equilibrium

Give

$$\hat{f}_i^{L} = \gamma_i x_i f_i \qquad (3 - 4)$$

From (3 - 1), (3 - 3) and (3 - 4) becomes

$$\hat{\phi}_i y_i P = \gamma_i x_i f_i \tag{3 - 5}$$

for low pressure :

$$\hat{\phi}_i y_i P = \gamma_i x_i P_i^{sat} \tag{3 - 6}$$

where we have omitted phase - identifying superscripts and P_i^{sat} stand for vapor pressure. The understanding is that $\hat{\phi}_i$, fugacity coefficient of component i in mixture applies to the vapor phase, whereas γ_i and f_i apply to the liquid phase. When all quantities are correctly evaluated at the equilibrium T and P, this equation is exact and entirely equivalent to equation (3 - 1).

Equilibrium constant (K_i)

For practical convenience, the equilibrium constant (K_i) has been introduced. Definition of equilibrium constant :

$$K_i \equiv \frac{y_i}{x_i} \tag{3 - 7}$$

from Eq.(3 - 5) we can write :

$$\frac{y_i}{x_i} = \frac{\gamma_i f_i}{\hat{\phi}_i P}$$

by definition of K_i, this equation becomes

$$K_i = \frac{y_i}{x_i} = \frac{\gamma_i f_i}{\hat{\phi}_i P} = \frac{\gamma_i P_i^{sat}}{\hat{\phi}_i P} \text{ (at low pressure)} \tag{3 - 8}$$

And from Eq.(3 - 1), (3 - 2) and (3 - 3) we can write :

$$\frac{y_i}{x_i} = \frac{\hat{\phi}_i^L}{\hat{\phi}_i^V}$$

by definition of K_i, this equation becomes

$$K_i = \frac{y_i}{x_i} = \frac{\hat{\phi}_i^L}{\hat{\phi}_i^V} \tag{3 - 9}$$

where fugacity coefficient can be evaluated from an equation of state (EOS) and activity coefficient can be evaluated from an activity coefficient model such as Wilson equation. So, the equilibrium constant (K_i) is depend on the property model used.

3.2 Fugacity Coefficient

The fugacity coefficient ($\hat{\phi}_i$) of a component i in the vapor phase is related to its mole fraction y_i in the vapor phase and the total pressure P by the fugacity coefficient :

$$\hat{\phi}_i \equiv \frac{\hat{f}_i^v}{y_i P} \tag{3-10}$$

The fugacity coefficient is a function of temperature, total pressure, and composition of the vapor phase; it can be calculated from volumetric data for the vapor mixture. For mixture containing m components, such data are often expressed in the form of an equation of state (EOS) explicit in the pressure

$$P = P(T, V, n_1, n_2, \ldots\ldots, n_m) \tag{3-11}$$

where V is the total volume having n_1 moles of 1, n_2 moles of 2, etc.

The fugacity coefficient can be determined using an equation of state (EOS) such as: virial equation, cubic equation of state.

3.2.1 Equations of State

Virial Equation of State

The Virial equation of state is a polynomial series in inverse volume which is explicit in pressure and can be derived from statistical mechanics :

$$P = \frac{RT}{V} + \frac{RTB}{V^2} + \frac{RTC}{V^3} + \ldots.. \tag{3-12}$$

The parameters B,C,... are called the second, third,...virial coefficients and are function only of temperature for a pure fluid. More often the virial equation is truncated to contain only the second virial coefficient. The virial equation may also be written as a power series in either V or P, so that truncation leads to two forms ; these are

$$Z = 1 + \frac{BP}{RT} \tag{3 - 13}$$

$$Z = 1 + \frac{B}{V} \tag{3 - 14}$$

The virial equation apply only to gases. For a pure vapor the virial coefficients are functions only of temperature; for a mixture they are also functions of composition. An important advantage of the virial equation is that there are theoretically valid relations between the virial coefficients of a mixture and its composition. These relations are:

$$B_{mixture}(T, y_1, \ldots, y_m) = \sum_{i=1}^{m}\sum_{j=1}^{m} y_i y_j B_{ij}(T) \tag{3 -15}$$

The individual coefficient B_{ij} are functions only of temperature and on components i and j where $B_{ij} = B_{ji}$ and y is the mole fraction. For binary mixture,

$$B_{mixture} = y_1^2 B_{11} + 2y_1y_2B_{12} + y_2^2 B_{22} \tag{3-16}$$

The fugacity coefficient ($\hat{\phi}_i$) is found from the thermodynamic relation:

$$\ln \hat{\phi}_i = \int_0^P \frac{\bar{Z}_i - 1}{P} dP \tag{3-17}$$

where $$\bar{Z}_i = \frac{P\bar{V}_i}{RT} \tag{3-18}$$

and the partial molar volume $\bar{V}_i$ is defined by

$$\bar{V}_i = \left(\frac{\partial V}{\partial n_i}\right)_{T,P,n_{j\neq i}} \tag{3-19}$$

In the equation (3-19), V is the total volume containing n_i moles of component i, n_j moles of component j, etc. The differentiation is carried out such that, in addition to temperature and pressure, all mole numbers (except n_i) are held constant.

When Equations (3-13) and (3-15) are substituted into Equation (3-17) we obtain

$$\ln \hat{\phi}_i = \left[2\sum_{j}^{m} y_j B_{ij} - B_{mixture}\right]\frac{P}{RT} \tag{3-20}$$

Equation (3-20) is applicable at low or moderate pressure, is used in the vapor mixture that does not contain one or more carboxylic acids.

Correlations for Second Virial Coefficients

For accurate values of B_{ii} and B_{jj} (the second virial coefficients of pure i and pure j) it is necessary to have accurate volumetric data for pure gas i and for pure gas j; for accurate values of B_{ij} it is necessary to have accurate volumetric data for gaseous mixtures of i and j. However, such data are usually not available, and it is necessary to estimate the desired second virial coefficients from correlation. These correlation vary considerable in their accuracy; in general, it is possible to estimate second virial coefficients of pure nonpolar gases with very good accuracy and second virial cross-coefficients B_{ij} for mixtures of nonpolar gases with good accuracy whenever components I and j have similar molecular size and volatility. Second virial coefficients of pure polar gases can be estimated with only fair accuracy, especially if the gas has a tendency to associate (e.g., by hydrogen bonding), and second virial cross-coefficients B_{ij} can be estimated only approximately if i or j (or both) is a polar component. Whenever reliable volumetric data are available for a pure or mixed gas, such data should be used in preference to virial coefficients obtained from correlations, especially in those cases where polar gases are concerned. Fortunately, vapor-liquid equilibria at normal pressures (say, up to 5 or 10 atmospheres) are not very sensitive to vapor-phase fugacity coefficients and thus virial coefficients of limited accuracy introduced little error into the phase equilibrium calculations. However, unless the pressure is very low, it is better to utilize even approximate values of the second virial coefficients than to assume ideal gas-phase behavior or the Lewis fugacity rule.

Pure Gases

For pure nonpolar gases an excellent corralation for B_{ii} has been given by Pitzer and Curl [15] based on a three-parameter theory of corresponding states.It has the form

$$\frac{P_{ci}B_{ii}}{RT_{ci}} = f_B^{(0)}(T_r) + \omega_i f_B^{(1)}(T_r) \tag{3-21}$$

where P_{ci} = critical pressure of i

T_{ci} = critical temperature of i

ω_i = acentric factor of i

T_R = reduced temperature, T/T_{ci}

The empirically determined functions $f_B^{(0)}(T_r)$ and $f_B^{(1)}(T_r)$ are

$$f_B^{(0)}(T_r) = 0.1445 - \frac{0.330}{T_r} - \frac{0.1385}{T_r^3} - \frac{0.0121}{T_r^3} \tag{3-22}$$

$$f_B^{(1)}(T_r) = 0.073 + \frac{0.46}{T_r} - \frac{0.50}{T_r^2} - \frac{0.097}{T_r^3} - \frac{0.0073}{T_r^8} \qquad (3\text{-}23)$$

Equation (3-21) gives excellent results for a large variety of nonpolar gases. For pure polar gases we have developed a new correlation based on an extended corresponding states theory. It has the form:

$$\frac{P_{ci}B_{ii}}{RT_{ci}} = f_B^{(0)}(T_r) + \omega_{Hi} f_B^{(1)}(T_r) + f_\mu(\mu_r, T_r) + \eta_i f_a(T_r) \qquad (3\text{-}24)$$

The symbol ω_{Hi} stands for the acentric factor of the polar component's homomorph. A homomorph of a polar molecule is a nonpolar molecule having approximately the same size and shape as those of the polar molecule. For example, the homomorph of acetone is isobutane.

The function $f_B^{(0)}(T_r)$ and $f_B^{(1)}(T_r)$ are the same as those given by Eqs. (3-22) and (3-23). The functions $f_\mu(\mu_{r,} T_r)$ depends on the reduced dipole moment

$$\mu_r = \frac{10^5 \mu_i^2 P_{ci}}{T_{ci}^2} \qquad (3\text{-}25)$$

where μ_i is the dipole moment of i in Debye. And the reduced temperature(T_r):

$$T_r = \frac{T}{T_{ci}}$$

where tempeature (T) is in degrees Kelvin.

$$\begin{aligned} f_\mu(\mu_r, T_r) = {} & -5.237220 + 5.665807 \ln \mu_r - 2.133816 (\ln \mu_r)^2 \\ & + 0.2525373 (\ln \mu_r)^3 + \frac{1}{T_r}[5.769770 - 6.181427 \ln \mu_r \\ & + 2.283270 (\ln \mu_r)^2 - 0.2649074 (\ln \mu_r)^3] \end{aligned} \qquad (3\text{-}26)$$

The association constant η_i is a term which reflects the tendency of a component (e.g., an alcohol) to associate with itself to form dimers. The association function $f_a(T_r)$ is given by

$$f_a(T_r) = \exp[6.6(0.7 - T_r)] \qquad (3\text{-}27)$$

The polar contributions of equation (3-26) and (3-27) are useful below a reduced temperature of 0.95 but should be neglected at higher temperatures where the polar interactions are small. If μ_r is less than 4, equation (3-26) is not applicable and the polar contributions should be ignored.

The Cross-Coefficient B_{ij} ($i \neq j$)

To estimate the cross-coefficients B_{ij}, the previously presented correlating equations for pure components are with suitable mixing rules for the various parameters.For the case where i and j are both nonpolar gases, equation (3-21), (3-22), and (3-23) give B_{ij} where P_{cij} replaces P_{ci}; and ω_{ij} replaces ω_i. The following mixing rules are recommended [15]:

$$T_{cij}=(T_{ci}T_{cj})^{1/2} \qquad (3\text{-}28)$$

$$\omega_{ij}=1/2(\omega_i+\omega_j) \qquad (3\text{-}29)$$

$$P_{cij} = 4T_{cij}\left[\frac{P_{ci}\nu_{ci}}{T_{ci}} + \frac{P_{cj}\nu_{cj}}{T_{cj}}\right] \Bigg/ (\nu_{ci}^{1/3} + \nu_{cj}^{1/3})^3 \qquad (3\text{-}30)$$

where ν_c is the critical volume.

These mixing rules appear to give good results wherever components i and j have similar molecular size and volatility. When components i and j are very dissimilar, empirical modification of the mixing rules may be required.

For the case where i is a polar molecule and j is nonpolar, Eqs. (3-21), (3-22), and (3-23) are used for B_{ij}; Eq. (3-28) used for T_{cij}; Eq. (3-31) is used for ω_{ij}:

$$\omega_{ij}=1/2(\omega_i+\omega_j) \qquad (3\text{-}31)$$

and equation (3-30) is used for P_{cij}.

For the case where both i and j are polar, equation (3-24) is used for B_{ij}. In equation (3-24) T_{ci} is replaced by T_{cij}; P_{ci} is replaced by P_{cij}; ω_{Hi} is replaced by ω_{Hij} and specific interaction constant η_i by η_{ij}. The reduced dipole moment, μ_r is given by

$$\mu_r = \frac{10^5 \mu_i \mu_j P_{cij}}{T_{cij}^2} \qquad (3\text{-}32)$$

The following mixing rules are used:

$$\omega_{Hij}=1/2(\omega_{Hi}+\omega_{Hj}) \qquad (3\text{-}33)$$

For T_{cij} use Eq. (3-28). For P_{cij} use Eq. (3-30) and

$$\eta_{ij} = \tfrac{1}{2}(\eta_i + \eta_j) \qquad (3\text{-}34)$$

Cubic equations of state

The term "cubic equation of state" implies an equation which, if expanded, would contain volume terms raised to either the first, second, or third power. Many of the common two-parameter cubic equations can be expressed by the equation

$$P = \frac{RT}{V-b} - \frac{a}{V^2 + ubV + wb^2} \tag{3-35}$$

An equivalent form of Eq.(3-35) is

$$Z^3 - (1 + B^* - uB^*)Z^2 + (A^* + wB^{*2} - uB^* - uB^{*2})Z - A^*B^* - wB^{*2} - wB^{*3} = 0 \tag{3-36}$$

where $$A^* = \frac{aP}{R^2T^2} \tag{3-37}$$

and $$B^* = \frac{bP}{RT} \tag{3-38}$$

Four well-known cubic equations are the van der Walls, Redlich-Kwong(RK), Soave Redlich-Kwong (SRK), and Peng-Robinson(PR) equations. For these four equations, u and w take on the integer values, a and b, that appear in Eq.(3-35) are shown in Table 3.1.

Application of cubic equation in calculation yields fugacity coefficient :

$$\ln\phi_i = \frac{b_i}{b}(Z-1) - \ln(Z-B^*) + \frac{A^*}{B^*\sqrt{u^2-4w}}\left(\frac{b_i}{b} - \delta_i\right)\ln\frac{2Z + B^*(u + \sqrt{u^2-4w})}{2Z + B^*(u - \sqrt{u^2-4w})} \tag{3-39}$$

where $$\frac{b_i}{b} = \frac{T_{ci}/P_{ci}}{\sum_j y_j T_{cj}/P_{cj}} \tag{3-40}$$

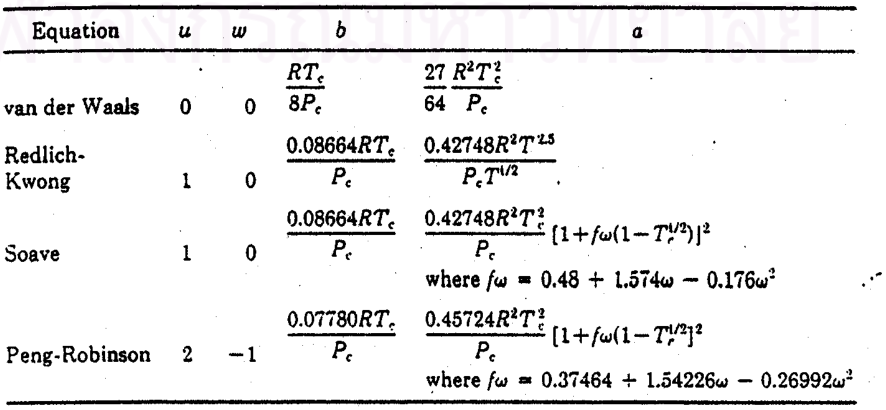
$$\delta_i = \frac{2a_j^{1/2}}{a}\sum_j x_j a_j^{1/2}(1-\bar{k}_{ij}) \tag{3-41}$$

if all $\bar{k}_{ij} = 0$, this reduce to

$$\delta_i = 2\left(\frac{a_i}{a}\right) \tag{3-42}$$

where u, w, a, b are shown in Table 3.1.

Table 3.1 Constants for Four Common Cubic Equation of State.[20]



Equation	u	w	b	a
van der Waals	0	0	$\frac{RT_c}{8P_c}$	$\frac{27}{64}\frac{R^2T_c^2}{P_c}$
Redlich-Kwong	1	0	$\frac{0.08664RT_c}{P_c}$	$\frac{0.42748R^2T^{2.5}}{P_cT^{1/2}}$
Soave	1	0	$\frac{0.08664RT_c}{P_c}$	$\frac{0.42748R^2T_c^2}{P_c}[1+f\omega(1-T_r^{1/2})]^2$ where $f\omega = 0.48 + 1.574\omega - 0.176\omega^2$
Peng-Robinson	2	−1	$\frac{0.07780RT_c}{P_c}$	$\frac{0.45724R^2T_c^2}{P_c}[1+f\omega(1-T_r^{1/2}]^2$ where $f\omega = 0.37464 + 1.54226\omega - 0.26992\omega^2$

3.3 Activity Coefficient

In a liquid mixture, all activity coefficients can be calculated by one of many equations such as: Wilson equation, van Laar equation, Margules equation or NRTL equation (called activity coefficient models).

3.3.2 Activity Coefficient Models

The popular activity coefficient models are : Wilson equation, van Laar equation, Margules equation, NRTL equation. For binary system, these equations are

Wilson equation :

$$\ln\gamma_1 = -\ln(x_1 + A_{12}x_2) + x_2\left[\frac{A_{12}}{x_1 + A_{12}x_2} - \frac{A_{21}}{A_{21}x_1 + x_2}\right] \qquad (3-43)$$

$$\ln\gamma_2 = -\ln(x_2 + A_{21}x_1) - x_1\left[\frac{A_{12}}{x_1 + A_{12}x_2} - \frac{A_{21}}{A_{21}x_1 + x_2}\right] \qquad (3-44)$$

where A_{12} , A_{21} = parameter

van Laar equation :

$$\ln\gamma_1 = \Lambda_{12}\left(\frac{\Lambda_{21}x_2}{\Lambda_{12}x_1 + \Lambda_{21}x_2}\right)^2 \qquad (3-45)$$

$$\ln\gamma_2 = \Lambda_{21}\left(\frac{\Lambda_{12}x_1}{\Lambda_{12}x_1 + \Lambda_{21}x_2}\right)^2 \qquad (3-46)$$

where Λ_{12} , Λ_{21} = parameter

Margules equation :

$$\ln\gamma_1 = x_2^2[\overline{A}_{12} + 2x_1(\overline{A}_{21} - \overline{A}_{12})] \qquad (3-47)$$

$$\ln\gamma_2 = x_1^2[\overline{A}_{21} + 2x_2(\overline{A}_{12} - \overline{A}_{21})] \qquad (3-48)$$

where $\overline{A}_{12}$, $\overline{A}_{21}$ = parameter

NRTL equation :

$$\ln\gamma_1 = x_2^2\left[\tau_{21}\left(\frac{G_{21}}{x_1 + x_2G_{21}}\right)^2 + \left(\frac{\tau_{12}G_{12}}{(x_2 + x_1G_{12})^2}\right)\right] \qquad (3 - 49)$$

$$\ln\gamma_2 = x_1^2\left[\tau_{12}\left(\frac{G_{12}}{x_2 + x_1G_{12}}\right)^2 + \left(\frac{\tau_{21}G_{21}}{(x_1 + x_2G_{21})^2}\right)\right] \qquad (3 - 50)$$

where $\tau_{12} = \frac{g_{12} - g_{22}}{RT}$ $\qquad \tau_{21} = \frac{g_{21} - g_{11}}{RT}$

$G_{12} = \exp(-\alpha_{12}\tau_{12})$ $\qquad G_{21} = \exp(-\alpha_{21}\tau_{21})$

$(g_{12} - g_{22})$, $(g_{21} - g_{11}) =$ parameter of components; $g_{12} = g_{21}$

$\alpha_{12} =$ nonrandomness parameter; $\alpha_{12} = \alpha_{21}$

3.4 Excess Properties

An excess property is defined as the difference between an actual property and the property that would be calculated at the same conditions of T, P, and x by the equations for an ideal solution.

$$\begin{aligned} M^E &= M - M^{id} \\ &= \sum x_iM_i(T,P) + \Delta M - M^{id} \end{aligned} \qquad (3\text{-}51)$$

where M^E and ΔM are the excess solution property and the property change of mixing, respectively. For internal energy (U), enthalpy (H), volume (V) and heat capacities (C_p and C_v), the ideal property, M^{id}, is

$$M^{id} = \sum x_iM_i \qquad (3\text{-}52)$$

For Gibbs free energy (G/RT) and entropy (S/R), the ideal property is

$$M^{id} = \sum x_iM_i - \sum x_i \ln x_i \qquad (3\text{-}53)$$

The entropy and entropy-related functions contain an ideal entropy of mixing term. The excess Gibbs free energy property, G^E, is related to the activity coefficients as:

$$\begin{aligned}\frac{G^E}{RT} &= \frac{\Delta G}{RT} - \sum x_i \ln x_i \\ &= \sum x_i \ln \hat{a}_i - \sum x_i \ln x_i \\ &= \sum x_i \ln \gamma_i\end{aligned} \qquad (3\text{-}54)$$

where $\hat{a}_i$ and γ_i are the activity and activity coefficient of component i.

The total derivertive of (G^E/RT) for a binary mixture is

$$d\left[\frac{G^E}{RT}\right] = \left[\frac{\partial(G^E/RT)}{\partial T}\right]_{P,x_i} dT + \left[\frac{\partial(G^E/RT)}{\partial P}\right]_{T,x_i} dP - \sum_{i=1}^{n}\left[\frac{\overline{G}^E}{RT}\right] dx_i \qquad (3\text{-}55)$$

$\overline{G}^E$: the partial molar Gibbs free energy of component i. The derivertive term, $\left[\frac{\partial(G^E/RT)}{\partial T}\right]_{P,x_i}$ can be related to the excess enthalpy by thermodynamic identities.

$$\left[\frac{\partial(G^E/RT)}{\partial T}\right]_{P,x} = \left[\frac{\partial(G^E/\partial T)}{T}\right]_{P,x} - \left[\frac{G^E}{T^2}\right] = \left[\frac{H^E}{T^2}\right] \qquad (3\text{-}56)$$

and

$$\left[\frac{G^E(T_2)}{RT_2}\right] = \left[\frac{G^E(T_1)}{RT_1}\right] - \int_{T_1}^{T_2}\left(\frac{H^E}{RT^2}\right) dT \qquad (3\text{-}57)$$

The excess Gibbs free energy at one temperature can be determined from G^E at another temperature by numerical integration using the measured excess enthalpies over a temperature range, We also can express activity coefficients in the form

$$\ln\gamma_1 = x_2^2\left[g^E + x_1\left(\frac{dg^E}{dx_1}\right)\right] \qquad (3\text{-}58)$$

$$\ln\gamma_2 = x_1^2\left[g^E - x_2\left(\frac{dg^E}{dx_1}\right)\right] \qquad (3\text{-}59)$$

where $g^E = \frac{G^E}{x_1 x_2 RT}$

Excess heat capacity C_p^E, and entropy at constant pressure S^E,are given by :

$$\left[\frac{\partial H^E}{\partial T}\right]_{x,P} = C_p^E \qquad (3\text{-}60)$$

$$\left[\frac{\partial G^E}{\partial T}\right]_{x,P} = -S^E \tag{3-61}$$

From thermodynamic relations, other excess properties can be derived :

$$U^E = H^E - PV^E \tag{3-62}$$

$$A^E = G^E - PV^E \tag{3-63}$$

H^E and G^E are determined under experimental conditions of constant pressure. The excess internal energy and the excess Helmholtz free energy from equations (3-62) and (3-63) are U_p^E and A_p^E. Most of the theoretical models (e.g. van Laar) used to explain the behavior of solutions are formulated with the assumption of zero volume of mixing.

3.4.1 Excess Gibbs Energy (G^E)

The excess Gibbs energy (G^E) is related to activity coefficient (γ_i). The basic relation is

$$\frac{G^E}{RT} = \sum x_i \ln\gamma_i \tag{3-64}$$

and

$$\ln\gamma_i = \frac{G^E}{RT} - \sum_{k\neq i} x_k \left(\frac{\partial(G^E/RT)}{\partial x_k}\right)_{T,P,x_{j\neq i,k}} \tag{3-65}$$

for binary mixtures,

$$\frac{G^E}{RT} = x_1\ln\gamma_1 + x_2\ln\gamma_2 \tag{3-66}$$

$$RT\ln\gamma_1 = G^E + (1-x_1)\left(\frac{\partial G^E}{\partial x_1}\right) \tag{3-67}$$

$$RT\ln\gamma_2 = G^E - x_1\left(\frac{\partial G^E}{\partial x_1}\right) \tag{3-68}$$

Correlation of excess Gibbs energies are empirical in form or based on semirational grounds. For binary mixtures the following general types of formulas are useful.

$$G^E = \alpha_1\alpha_2 f(\alpha_1) \tag{3-69}$$

$$G^E = x_1x_2 f(x_1) \tag{3-70}$$

in terms of (α) volume fractions and (x) mole fractions, respectively. From this relation the activity coefficient model such as: Wilson equation, Van Laar equation, Margules equation and NRTL equation can be represented as follows.

Wilson equation:

$$\frac{G^E}{RT} = -x_1 \ln(x_1 + A_{12}x_2) - x_2 \ln(A_{21}x_2 + x_1) \tag{3-71}$$

where A_{12} , A_{21} = parameter

Van Laar equation:

$$\frac{G^E}{RT} = \frac{1}{\left(\frac{1}{\Lambda_{12}x_1} + \frac{1}{\Lambda_{21}x_2}\right)} \tag{3-72}$$

where Λ_{12} , Λ_{21} = parameter

Margules equation:

$$\frac{G^E}{RT} = x_1x_2(\bar{A}_{21}x_1 + \bar{A}_{12}x_2) \tag{3-73}$$

where $\bar{A}_{12}$, $\bar{A}_{21}$ = parameter

NRTL equation:

$$\frac{G^E}{RT} = x_1x_2\left(\frac{\tau_{21}G_{21}}{x_1 + G_{21}x_2} + \frac{\tau_{12}G_{12}}{G_{12}x_1 + x_2}\right) \tag{3-74}$$

where $\tau_{12} = \frac{g_{12} - g_{22}}{RT}$ $\qquad \tau_{21} = \frac{g_{21} - g_{11}}{RT}$

$G_{12} = \exp(-\alpha_{12}\tau_{12})$ $\qquad G_{21} = \exp(-\alpha_{21}\tau_{21})$

$(g_{12} - g_{22})$, $(g_{21} - g_{11})$ = parameter of components; $g_{12} = g_{21}$

α_{12} = nonrandomness parameter; $\alpha_{12} = \alpha_{21}$

3.4.2 Excess Enthalpy (H^E)

The excess enthalpy (H^E) is related to the activity coefficient (γ_i) by following relationship.

$$H^E = -RT^2 \sum x_i \left(\frac{\partial \ln \gamma_i}{\partial T} \right)_{P,x} \tag{3-75}$$

and the activity coefficient (γ_i) can be represented in Gibbs energy (G^E/RT) term, so equation (3-61) becomes

$$H^E = -RT^2 \sum x_i \left(\frac{\partial (G^E / RT)}{\partial T} \right)_{P,x} \tag{3-76}$$

In the previous section is shown the relationship of Gibbs energy (G^E/RT) term in various equations. Then (G^E/RT) term in equation (3-62) can be replaced such as;

Wilson equation:

$$H^E = x_1 x_2 \left(\frac{\lambda_{12} A_{12}}{x_1 + A_{12} x_2} + \frac{\lambda_{21} A_{21}}{A_{21} x_1 + x_2} \right) \tag{3-77}$$

where $A_{12} = \frac{V_2}{V_1} \exp(-\lambda_{12} / RT)$

$A_{21} = \frac{V_1}{V_2} \exp(-\lambda_{21} / RT)$

$V_i =$ molar volume of pure liquid component i

3.5 Enthalpy (H)

In modern separation design, a significant part of many phase-equilibrium calculation is the mathematical representation of pure-component and mixture enthalpies. Enthalpy estimate is important not only for determination of heat loads, but also for adiabatic flash and distillation computations. Further, mixture enthalpy data, when available, are useful for extending vapor-liquid equilibria to higher (or lower) temperatures, through the Gibbs-Helmholtz equation. The general form of the Gibbs-Helmholtz equation is

$$\left(\frac{\partial g/T}{\partial l/T}\right)_{P,x} = h \tag{3-78}$$

where x refers to the composition. If we apply this equation to a liquid mixture, it is convenient to rewrite the equation in the form

$$\left(\frac{\partial g^{E}/T}{\partial l/T}\right)_{P,x} = h^{E} \tag{3-79}$$

where g^{E} is the molar excess Gibbs energy of the mixture and h^{E} is the molar excess enthalpy, also called the enthalpy of mixing.

The enthalpy of the real vapor is found from zero-pressure heat capacities and from the Virial equation of state for non-associated species or, for vapors containing highly dimerized vapors (e.g. organic acids). For pure components, liquid-phase enthalpies (relative to the ideal vapor) are found from differentiation at the zero-pressure standard-state fugacities; these, in turn, are determined from vapor-pressure data, from vapor-phase corrections and liquid-phase densities. If good experimental data are used to determine the standard-state fugacity, the derivative gives enthalpies of liquids to nearly the same precision as that obtained with calorimetric data, and provides reliable heats of vaporization. The enthalpy can be calculated by one of the following methods.

3.5.1 Calculating from an Equation of State (EOS)

For a real vapor mixture that phase change from liquid phase to vapor phase, there is a deviation from the ideal enthalpy that can be calculated from an equation of state and enthalpy of liquid phase change to vapor phase can be calculated from latent heat or heat of vaporization (ΔH_{v}). The enthalpy of real vapor (H) is given by

$$H_{v} = H^{id} + \Delta H' + (H^{sat,liq} - H^{sat,vap}) - H_{L} \tag{3-80}$$

where H^{id} is the enthalpy of an ideal vapor mixture.

$\Delta H'$ is the residual enthalpy of a mixture.

$H^{sat,liq} - H^{sat,vap}$ is enthalpy of phase change from liquid to vapor.

H_{L} is enthalpy of liquid phase.

For the enthalpy of a pure ideal vapor (H_{i}^{id}) at temperature T, relative to some reference temperature T_0 is given by

$$H_i^{id} = \int_{T_0}^{T} C_{pi}^{*} dT \tag{3-81}$$

The heat capacity (C^{*}_{pi}) of an ideal gas is function of temperature, In this work it is expressed by the empirical relation [16]

$$C_{pi}^{*} = D_{1i} + \frac{D_{2i}}{T} + D_{3i}T + D_{4i}\ln T \tag{3-82}$$

where D_{ij} are constants for each pure component i.

C^{*}_{pi} is in J/mole-K and temperature (T) in K.

Substitution of equation (3-66) into (3-65) and integration gives

$$\begin{aligned} H^{id} = \sum_{i=1}^{m} y_i [\, & D_{1i}(T - T_0) + D_{2i}\ln(T/T_0) + D_{3i}(T^2 - T_0^2)/2 \\ & + D_{4i}(T\ln T - T_0\ln T_0 + T_0 - T)\,] \end{aligned} \tag{3-83}$$

And the residual enthalpy ($\Delta H'$) is given

$$\Delta H' = H^{id} - H \tag{3-84}$$

This equation will be developed in term of equation of state (EOS).

$$\begin{aligned} \Delta H' &= H^{id} - H \\ &= \int_0^P \left[\left(\frac{\partial H^{id}}{\partial P}\right)_T - \left(\frac{\partial H}{\partial P}\right)_T \right] dP \\ &= \int_0^p \left[T\left(\frac{\partial V}{\partial T}\right)_P - V \right] dP \end{aligned} \tag{3-85}$$

Equation of state explicit in volume are of the forms:

$$V = V(P,T) \text{ or } V = (RT/P)Z(P,T) \tag{3-86}$$

$$= RT^2 \int_0^P \left(\frac{\partial Z}{\partial T}\right)_P \frac{dP}{P} \tag{3-87}$$

From the Virial equation of state :

$$Z = 1 + \frac{B}{V} + \frac{C}{V^2} + \ldots. \tag{3-88}$$

$$= 1 + B'P + C'P^2 + \ldots. \tag{3-89}$$

$$B' = \frac{B}{RT} \tag{3-90}$$

$$C' = (C - B^2)/(RT)^2 \tag{3-91}$$

$$\frac{dB'}{dT} = \frac{1}{RT}\left(\frac{dB}{dT} - \frac{B}{T}\right) \tag{3-92}$$

$$\frac{dC'}{dT} = \left(\frac{1}{RT}\right)^2\left(\frac{B^2 - C}{T} + \frac{dC}{dT} - 2B\frac{dB}{dT}\right) \tag{3-93}$$

$$\Delta H' = H^{id} - H = RT^2\left[P\frac{dB'}{dT} + \frac{P^2}{2}\frac{dC'}{dT} + ...\right] \tag{3-94}$$

$$= PT\left(\frac{dB}{dT} - \frac{B}{T}\right) + \frac{P^2}{2R}\left[\frac{B^2 - C}{T} + \frac{dC}{dT} - 2B\frac{dB}{dT} + ...\right] \tag{3-95}$$

With the Pitzer-Curl correlation[20] for B :

$$\begin{aligned}\Delta H' = H^{id} - H = RT_cP_r\ [&-(0.1445 + 0.073\omega) + (0.660 - 0.92\omega)/T_r \\ &+ (0.4155 + 1.50\omega)/T_r^2 + (0.0484 + 0.388\omega)/T_r^3 \\ &+ 0.0657\omega/T_r^8\ ]\end{aligned} \tag{3-96}$$

For mixture :

$$\begin{aligned}\Delta H' = H^{id} - H = R\sum_{i=1}^{m} T_{ci}P_{ri}\ [&-(0.1445 + 0.073\omega_i) + (0.660 - 0.92\omega_i)/T_{ri} \\ &+ (0.4155 + 1.50\omega_i)/T_{ri}^2 + (0.0484 + 0.388\omega_i)/T_{ri}^3 \\ &+ 0.0657\omega_i/T_{ri}^8\ ]\end{aligned} \tag{3-97}$$

For the latent heat or heat of vaporization of component i (ΔH_{vi})[1] can be calculated from slope of graph of $\ln P^{sat}$ & T. The latent heat (ΔH_{vi}) is the slope of graph multiply by gas constant (R).

$$\Delta H_{vi} = (\text{slope of graph } \ln P^{sat} \text{ \& T}) \times R \tag{3-98}$$

where R=8.31451 J/mol-K.

For mixture the enthalpy of phase change is :

$$H^{sat,liq} - H^{sat,vap} = -\sum_{i=1}^{m} x_i \Delta H_{vi} \tag{3-99}$$

Substitution of equation (3-83), (3-97) and equation (3-99) into equation (3-80) give :

The enthalpy (H_v) of real vapor mixture[16] is

$$H_v = \sum_{i=1}^{m} y_i [\, D_{1i}(T - T_0) + D_{2i}\ln(T/T_0) + D_{3i}(T^2 - T_0^2)/2 + D_{4i}(T\ln T - T_0\ln T_0 + T_0 - T)\,]$$

$$- R\sum_{i=1}^{m} T_{ci}P_{ri}\,[\,-(0.1445 + 0.073\omega_i) + (0.660 - 0.92\omega_i)/T_{ri} + (0.4155 + 1.50\omega_i)/T_{ri}^{2}$$

$$+ (0.0484 + 0.388\omega_i)/T_{ri}^{3} + 0.0657\omega_i/T_{ri}^{8}\,] - \sum_{i=1}^{m} x_i \Delta H_{vi} - H_L \qquad (3\text{-}100)$$

3.5.2 Calculating from Activity Coefficient (γ_i)

The enthalpy can be calculated from activity coefficient (γ_i). Since the activity coefficient (γ_i) is related to the excess enthalpy (H^E) that is described in section 3.4.2. The enthalpy of liquid mixture (H_L) is given by

$$H_L = H^{id} + \sum_{i=1}^{m} x_i \overline{H}_i \qquad (3\text{-}101)$$

where H^{id} is given by Eq.(3-83) with y's replaced by x's. Here $\overline{H}_i$ is the partial molar enthalpy of component i, at temperature T, pressure P, and composition x, relative to the molar enthalpy of pure ideal vapor i, at the same temperature. The partial molar enthalpy for every component i, is found from an appropriate form of the Gibbs-Helmholtz equation

$$\left(\frac{\partial \ln \hat{f}_i^{L}}{\partial T}\right)_{P,x} = -\frac{\overline{H}_i}{RT^{2}} \qquad (3\text{-}102)$$

where in the liquid mixture, $\hat{f}_i^{L}$ is the fugacity of component i.

$$f_i^{L} = \gamma_i^{(po)} x_i f_i^{(po)} \exp\left(\frac{\overline{V}_i P}{RT}\right) \qquad (3\text{-}103)$$

For condensable components, $f_i^{(po)}$ is the fugacity of pure liquid i, at temperature T corrected to zero pressure.

Substitution of equation (3-103) into equation (3-101) yields

$$H_L = H^{id} - \sum_{i=1}^{m} x_i RT^2 \left(\frac{\partial \ln \gamma_i^{(po)}}{\partial T}\right)_{P,x} - \sum_{i=1}^{m} x_i RT^2 \left(\frac{d\ln f_i^{(po)}}{dT}\right)_{pure} + \sum_{i=1}^{m} x_i P\left(\overline{V}_i - T\frac{d\overline{V}_i}{dT}\right) \qquad (3\text{-}104)$$

When attention is confined to moderate pressures, the last term in equation (3-104) can be neglected. The first term in equation (3-104) is given by equation (3-83), with x's replacing y's. In equation (3-104), the third term is much more important than the second term. The third term gives the enthalpy of the ideal liquid mixture (corrected to zero pressure) relative to that of the ideal vapor at the same temperature and composition. The second term gives the excess enthalpy, i.e. the liquid-phase enthalpy of mixing; often little basis exists for evaluation of this term, but fortunately its contribution to total liquid enthalpy is usually not large. For pure liquids the standard-state fugacity is represented by

$$\ln f_i^{(po)} = C_{1i} + \frac{C_{2i}}{T} + C_{3i}T + C_{4i}\ln T + C_{5i}T^2 \tag{3-105}$$

where the C_i's are constants for liquid i. These constants are determined primarily from vapor-pressure data and secondarily, from vapor-phase and liquid-phase volumetric data. Differentiation of equation (3-105) gives

$$\sum_{i=1}^{m} x_i RT^2\left(\frac{d\ln f_i^{(po)}}{dT}\right) = R\sum_{i=1}^{m} x_i(-C_{2i} + C_{3i}T^2 + C_{4i}T + 2C_{5i}T^3) \tag{3-106}$$

Equation (3-106) provides the third term in equation (3-104). The molar excess enthalpy H^E is related to the derivatives of the activity coefficients with respect to temperature according to

$$H^E = -RT^2\sum_{i=1}^{m} x_i\left(\frac{\partial \ln\gamma_i^{(po)}}{\partial T}\right)_{P,x} \tag{3-107}$$

Since the excess enthalpy (H^E) is related to the activity coefficient (γ_i) such as Wilson model that give equation (3-77). For binary mixture[20] gives

$$H^E = x_1x_2\left(\frac{\lambda_{12}A_{12}}{x_1 + A_{12}x_2} + \frac{\lambda_{21}A_{21}}{A_{21}x_1 + x_2}\right) \tag{3-108}$$

Substitution of Eq. (3-83), Eq. (3-106) and Eq. (3-107) into Eq. (3-104) yields the enthalpy of liquid mixture[16] is

$$\begin{aligned} H_L = {}& \sum_{i=1}^{m} x_i[D_{1i}(T-T_0) + D_{2i}\ln(T/T_0) + D_{3i}(T^2-T_0^2)/2 + D_{4i}(T\ln T - T_0\ln T_0 + T_0 - T)] \\ & -R\sum_{i=1}^{m} x_i(-C_{2i} + C_{3i}T^2 + C_{4i}T + 2C_{5i}T^3) + H^E \end{aligned} \tag{3-109}$$

For binary mixture the excess enthalpy (H^E) is substituted by equation (3-108). Normally, in the experimental data is referenced by the reference state. So, the enthalpy of reference state is used. The enthalpy at reference state ($H_{L,ref}$) can be calculated from equation (3-109) then use temperature and pressure at reference state.

At the end the enthalpy of liquid mixture is

$$H_L = \sum_{i=1}^{m} x_i [D_{1i}(T - T_0) + D_{2i}\ln(T/T_0) + D_{3i}(T^2 - T_0^2)/2 + D_{4i}(T\ln T - T_0\ln T_0 + T_0 - T)]$$

$$-R\sum_{i=1}^{m} x_i(-C_{2i} + C_{3i}T^2 + C_{4i}T + 2C_{5i}T^3) + H^E - H_{L,ref} \qquad (3\text{-}110)$$

3.6 Vapor pressure model

Various vapor pressure models[19] are available. Each model have different accuracy.

Clausius-Clapeyron equation:

$$\ln P_{vp} = A - \frac{B}{T} \qquad (3\text{-}111)$$

where P_{vp} = vapor pressure (bar)

T = temperature (K)

A,B = constants

It is a fairly good relation for approximating vapor pressure over small temperature intervals. Except near the critical point.

Pitzer equation:

$$\ln P_{vpr} = f^{(0)}(T_r) + \omega f^{(1)}(T_r) \qquad (3\text{-}112)$$

The functions $f^{(0)}$ and $f^{(1)}$ have been expressed as follows :

$$f^{(0)} = 5.92714 - \frac{6.09648}{T_r} - 1.28862\ln T_r + 0.169347T_r^6 \qquad (3\text{-}113)$$

$$f^{(1)} = 15.2518 - \frac{15.6875}{T_r} - 13.4721\ln T_r + 0.43577T_r^6 \qquad (3\text{-}114)$$

where P_{vp} = vapor pressure (bar)

ω = acentric factor

T_r = T/T_c = reduced temperature (K)

T_c = critical temperature (K)

Antoine vapor pressure correlation:

$$\ln P_{vp} = A - \frac{B}{T + C} \tag{3-115}$$

where P_{vp} = vapor pressure (bar)

T = temperature (K)

A,B,C = constants

Antoine proposed a simple modification of Clausious equation (3-111) which has been widely used over limited temperature ranges. The applicable temperature range is not large and in most instances corresponds to a pressure interval of about 0.01 to 2 bar. The Antoine equation should never be used outside the stated temperature limits.

Gomez-Thodos vapor pressure equation:

Gomez-Nieto and Thodos presented the following equation for estimating vapor pressure:

$$\ln P_{vpr} = \beta\left[\frac{1}{T_r^m} - 1\right] + \gamma\left[T_r^7 - 1\right] \tag{3-116}$$

where P_{vpr}= vapor pressure at reduced temperature (bar)

$T_r = T/T_c$ = reduced temperature (K)

T_c = critical temperature (K)

This equation is necessarily satisfied at the critical point. The normal boiling point provides an additional equation which relates the constants β, γ, and m to each other. This leads to

$$\gamma = ah + b\beta \tag{3-117}$$

where

$$a = \frac{1 - 1/T_{br}}{T_{br}^7 - 1} \tag{3-118}$$

$$b = \frac{1 - 1/T_{br}^m}{T_{br}^7 - 1} \tag{3-119}$$

$$h = T_{br}\frac{\ln(P_c/1.01325)}{1 - T_{br}} \tag{3-120}$$

T_{br}= boiling point at reduced temperature (K)

P_c = critical pressure (bar)

Compounds are devided into three classes: non-polar, polar, and hydrogen-bonded compounds. The procedure for determining β, γ, and m is different for each class.

For nonpolar compounds (both organic and inorganic)

$$\beta = 4.26700 - \frac{221.79}{h^{2.5}\exp 0.0384h^{2.5}} + \frac{3.8126}{\exp(2272.44/h^{3})} + \Delta^{*} \qquad (3\text{-}121)$$

$$m = 0.78425\exp(0.089315h) - \frac{8.5217}{\exp(0.74826h)} \qquad (3\text{-}122)$$

where Δ^{*} = 0 except the He (Δ^{*} = 0.41815), H_2(Δ^{*} = 0.19904) and Ne(Δ^{*} = 0.02319).

γ is obtained from equation (3-117)

For polar compounds that do not hydrogen-bond (this class includes ammonia and acetic acid),

$$m = 0.466T_c^{0.166} \qquad (3\text{-}123)$$

$$\gamma = 0.08594\exp(7.462x10^{-4}T_c) \qquad (3\text{-}124)$$

For hydrogen-bonding compounds (water and alcohol)

$$m = 0.466M^{0.29}T_c^{0.72} \qquad (3\text{-}125)$$

$$\gamma = \frac{2.464}{M}\exp(9.8x10^{-6}MT_c) \qquad (3\text{-}126)$$

For these last two categories of compounds, β is obtained from equation (3-117) i.e.,

$$\beta = \frac{\gamma}{b} - \frac{ah}{b} \qquad (3\text{-}127)$$

Vapor pressure estimation with two reference fluid:

$$\ln P_{vpr} = \ln P_{vpr}^{(R1)} + (\ln P_{vpr}^{(R2)} - \ln P_{vpr}^{(R1)})\frac{\omega - \omega^{(R1)}}{\omega^{(R2)} - \omega^{(R1)}} \qquad (3\text{-}128)$$

where P_{vpr} = vapor pressure at reduced temperature (bar)

ω = acentric factor

The superscripts R1 and R2 refer to the two reference substances. In this equation, all vapor pressures are calculated at the reduced temperature of the substance whose vapor pressure is being predicted.

Wagner equation:

$$\ln\left(\frac{P_{vp}}{P_c}\right) = (1-\tau)^{-1}\left[A\tau + B\tau^{1.5} + C\tau^{3} + D\tau^{6}\right] \qquad (3\text{-}129)$$

where $\tau = 1 - T_r$

P_{vp} = vapor pressure (bar)

T_r = T/T_c = reduced temperature (K)

T_c = critical temperature (K)

A, B, C, D = constants

This is the simplest form which arises from Wagner’s analysis; it has come to be referred to as the Wagner equation, even though a more complex form is superior for water, ammonia, and oxygen. In all situations in which a form of it was compared to other vapor pressure equations, the Wagner equation was selected as the best equation.

Frost-Kalkwarf-Thodos equation:

$$\ln P_{vp} = A - \frac{B}{T} + C \ln T + \frac{(D)(P_{vp})}{T^2} \qquad (3\text{-}130)$$

where P_{vp} = vapor pressure (bar)

T = temperature (K)

A, B, C, D = constants

This equation can be used when Wagner’s constants were not available for a particular compound.

CHAPTER 4

ANALYSING PROCEDURE

4.1 Experimental Data

4.1.1 Vapor-Liquid Equilibrium (VLE) Data

Vapor-liquid equilibrium data of ethanol+water system is from research of Kiyofumi Kurihara, Tsuyoshi Minoura, Kouichi Takeda and Kazuo Kojima[10]. The equilibrium temperature was measured with a calibrated platinum resistance thermometer with an accuracy of ±0.01 K. The pressure in the still was determined by the bubble point of water referring to the vapor pressure data on water (Bridgeman and Aldrich, 1964). The accuracy was estimated to be ±0.03 kPa.

Vapor and liquid samples were analyzed with a Simazu gas chromatograph type GC-8AIT equipped with a thermal conductivity cell. Porapak QS was used as the column packing and helium as the carrier gas. The compositions were determined by the relative area method with an accuracy of ±0.001 mole fraction.

The activity coefficients, γ_i, are presented in the Table4.1 were evaluated by the following equation [10]:

$$\phi_i P y_i = \gamma_i P_i^S \phi_i^S \exp\left[v_i^L (P - P_i^S)/RT\right] \tag{4-1}$$

where ϕ_i and ϕ_i^S are the fugacity coefficients of component i in the mixture and the pure vapor, respectively. They were calculated using the second virial coefficients. The liquid molar volumes v_i^L calculated by the modified Rackett equation. The vapor pressures of the pure components, P_i^S, were calculated from the Antoine equation.

The Antoine constants were determined from the vapor pressure data of the pure components measured. The average relative deviations between the values calculated by the Antoine equation and experimental values are less than 0.01% in all cases.

Table 4.1 Isothermal vapor-liquid equilibrium data of ethanol(1)+water(2) at 323.15K.[10]

P(kPa)	x_1	y_1	γ_1	γ_2	P(kPa)	x_1	y_1	γ_1	γ_2
20.333	0.0874	0.4341	3.4513	1.0187	28.448	0.6242	0.7205	1.1148	1.7106
20.904	0.0967	0.4549	3.3591	1.0192	28.711	0.6697	0.7434	1.0817	1.8037
22.796	0.1411	0.5120	2.8214	1.0463	28.828	0.6868	0.7523	1.0716	1.8439
23.663	0.1756	0.5372	2.4675	1.0731	29.195	0.7586	0.794	1.0366	2.0159
24.336	0.2065	0.5562	2.2331	1.0995	29.253	0.7811	0.8081	1.0266	2.0754
24.570	0.2253	0.5636	2.0935	1.1180	29.506	0.8299	0.8429	1.0129	2.1990
25.024	0.2552	0.5761	1.9235	1.1505	29.487	0.8454	0.8555	1.0119	2.2319
25.436	0.2856	0.5890	1.7856	1.1822	29.680	0.8559	0.8639	1.0090	2.2551
25.815	0.3133	0.6008	1.6845	1.2124	29.478	0.8638	0.8699	1.0067	2.2808
26.259	0.3535	0.6133	1.5497	1.2689	29.798	0.8713	0.8769	1.0067	2.2856
26.481	0.3773	0.6226	1.4861	1.2697	29.517	0.8801	0.8849	1.0063	2.2957
26.694	0.3999	0.6311	1.4325	1.3258	29.538	0.8911	0.8948	1.0057	2.3121
26.898	0.4258	0.6397	1.3788	1.3637	29.531	0.9031	0.9065	1.0051	2.3094
27.284	0.4691	0.6563	1.2973	1.4273	29.56	0.9136	0.9151	1.0039	2.3544
27.535	0.4987	0.6660	1.2495	1.4825	29.566	0.9263	0.9273	1.0035	2.3644
27.701	0.5218	0.6741	1.2158	1.5257	29.558	0.9344	0.9337	1.0014	2.4221
27.881	0.5421	0.6840	1.1950	1.5551	29.558	0.9480	0.9470	1.0011	2.4432
28.101	0.5692	0.6971	1.1688	1.5971	29.548	0.9528	0.9512	1.0001	2.4777
28.216	0.5907	0.7050	1.1436	1.6439					

Table 4.2 Isothermal vapor-liquid equilibrium data of ethanol(1)+water(2) at 328.15K.[10]

P(kPa)	x_1	y_1	γ_1	γ_2	P(kPa)	x_1	y_1	γ_1	γ_2
27.774	0.1161	0.4841	3.1244	1.0261	36.779	0.7174	0.7667	1.0533	1.9244
29.017	0.1445	0.5123	2.7731	1.0470	36.812	0.7276	0.7714	1.0458	1.9581
31.391	0.2338	0.5712	2.0638	1.1119	36.973	0.7558	0.7937	1.0402	1.9804
31.767	0.2506	0.5760	1.9644	1.1375	37.172	0.7979	0.8211	1.0246	2.0872
32.475	0.2938	0.5923	1.7605	1.1866	37.223	0.8165	0.8340	1.0184	2.1363
33.048	0.3306	0.6058	1.6278	1.2318	37.307	0.8334	1.8470	1.0154	2.1741
33.350	0.3551	0.6106	1.5411	1.2745	37.325	0.8486	0.8554	1.0136	2.1901
33.611	0.3777	0.6191	1.4803	1.3022	37.352	0.8502	0.8595	1.0112	2.2235
34.012	0.4123	0.6294	1.3946	1.3576	37.378	0.8616	0.8688	1.0093	2.2493
34.343	0.4470	0.6465	1.3338	1.3898	37.393	0.8714	0.8775	1.0083	2.2614
34.519	0.4598	0.6557	1.3216	1.3929	37.395	0.8798	0.8848	1.0070	2.2757
35.017	0.5127	0.6682	1.2249	1.5096	37.416	0.8854	0.8891	1.0061	2.2992
35.215	0.5273	0.6801	1.2188	1.5091	37.415	0.8925	0.8946	1.0042	2.3297
35.507	0.5541	0.6845	1.1768	1.5908	37.421	0.9002	0.9019	1.0039	2.3363
35.516	0.5626	0.6874	1.1642	1.6073	37.425	0.9131	0.9130	1.0020	2.3808
36.055	0.6194	0.7138	1.1142	1.7173	37.437	0.9342	0.9331	1.0012	2.4189
36.530	0.6841	0.7480	1.0706	1.8465	37.412	0.9566	0.9550	1.0000	2.4662

Table 4.3 Isothermal vapor-liquid equilibrium data of ethanol(1)+water(2) at 333.15K.[10]

P(kPa)	x_1	y_1	γ_1	γ_2	P(kPa)	x_1	y_1	γ_1	γ_2
31.647	0.0742	0.4130	3.7957	1.0037	45.881	0.6764	0.7468	1.0813	1.7974
34.540	0.1071	0.4742	3.2893	1.0172	46.218	0.7156	0.7674	1.0577	1.8931
36.840	0.1511	0.5196	2.7208	1.0425	46.338	0.7347	0.7834	1.0542	1.8951
37.611	0.1705	0.5326	2.5221	1.0597	46.547	0.7656	0.7968	1.0335	2.0218
38.387	0.1899	0.5473	2.3738	1.0726	46.868	0.8246	0.8395	1.0176	2.1504
38.999	0.2133	0.5587	2.1909	1.0939	46.915	0.8253	0.8477	1.0153	2.1756
40.175	0.2606	0.5814	1.9209	1.1373	46.998	0.8538	0.8616	1.0113	2.2317
41.230	0.3168	0.6006	1.6741	1.2052	46.987	0.8646	0.8715	1.0099	2.2572
42.157	0.3813	0.6209	1.4693	1.2918	47.020	0.8823	0.8860	1.0067	2.2855
42.635	0.4036	0.6316	1.4276	1.3170	47.045	0.8873	0.8908	1.0070	2.2878
43.368	0.4548	0.6502	1.3260	1.3917	47.048	0.8966	0.8987	1.0054	2.3137
43.730	0.4794	0.6688	1.3043	1.3917	47.060	0.9091	0.9095	1.0037	2.3524
43.756	0.4808	0.6682	1.3001	1.3988	47.055	0.9154	0.9151	1.0029	2.3712
44.336	0.5298	0.6788	1.2140	1.5151	47.055	0.9206	0.9195	1.0020	2.3957
44.447	0.5390	0.6887	1.2136	1.5017	47.044	0.9255	0.9242	1.0015	2.4039
44.935	0.5800	0.7070	1.1700	1.5687	47.026	0.9458	0.9444	1.0010	2.4238
45.282	0.6141	0.7175	1.1299	1.6590	47.039	0.9479	0.9467	1.0015	2.418
45.557	0.6417	0.7333	1.1115	1.6975	46.994	0.9583	0.9562	0.9997	2.4807

Table4.4 Isobaric vapor-liquid equilibrium data of ethanol(1)+water(2) at 101.3 kPa.

Temperature (K)	Mole fraction (x_1)	Mole fraction (y_1)	Activity coefficient (γ_1)	Activity coefficient (γ_2)
362.19	0.056	0.366	4.434	1.004
359.26	0.091	0.448	3.705	1.016
356.33	0.189	0.539	2.386	1.067
354.89	0.286	0.582	1.795	1.164
354.46	0.323	0.600	1.664	1.196
354.41	0.331	0.605	1.640	1.197
353.59	0.419	0.627	1.385	1.346
352.85	0.512	0.666	1.237	1.479
352.16	0.620	0.712	1.120	1.686
351.74	0.704	0.759	1.068	1.844
351.70	0.715	0.764	1.060	1.879
351.41	0.798	0.818	1.028	2.072
351.37	0.843	0.851	1.014	2.188
351.37	0.847	0.854	1.013	2.200
351.36	0.849	0.856	1.013	2.200
351.34	0.884	0.886	1.008	2.270
351.33	0.908	0.907	1.005	2.333
351.33	0.922	0.920	1.003	2.373

4.1.2 Enthalpy Data

Figure 4.1 gives an enthalpy-concentration diagram for ethanol(1)+water(2) at 1atm. The reference enthalpy is defined as that of the pure liquid at 0 °C and 1atm. And Figure 4.2 also gives an enthalpy-concentration diagram for ethanol(1)+water(2) at 1atm. The reference enthalpy is defined as that of the pure liquid at 0 °C and 1atm. The straight slanted lines are tie lines relating vapor compositions to liquid compositions at equilibrium. The nearly horizontal linear at the bottom of the figure represent isotherms for subcooled liquid. The nearly horizontal lines at the top represent isotherms for the superheated vapor. Reference state is enthalpies of liquid water and ethyl alcohol at 0°C are zero.

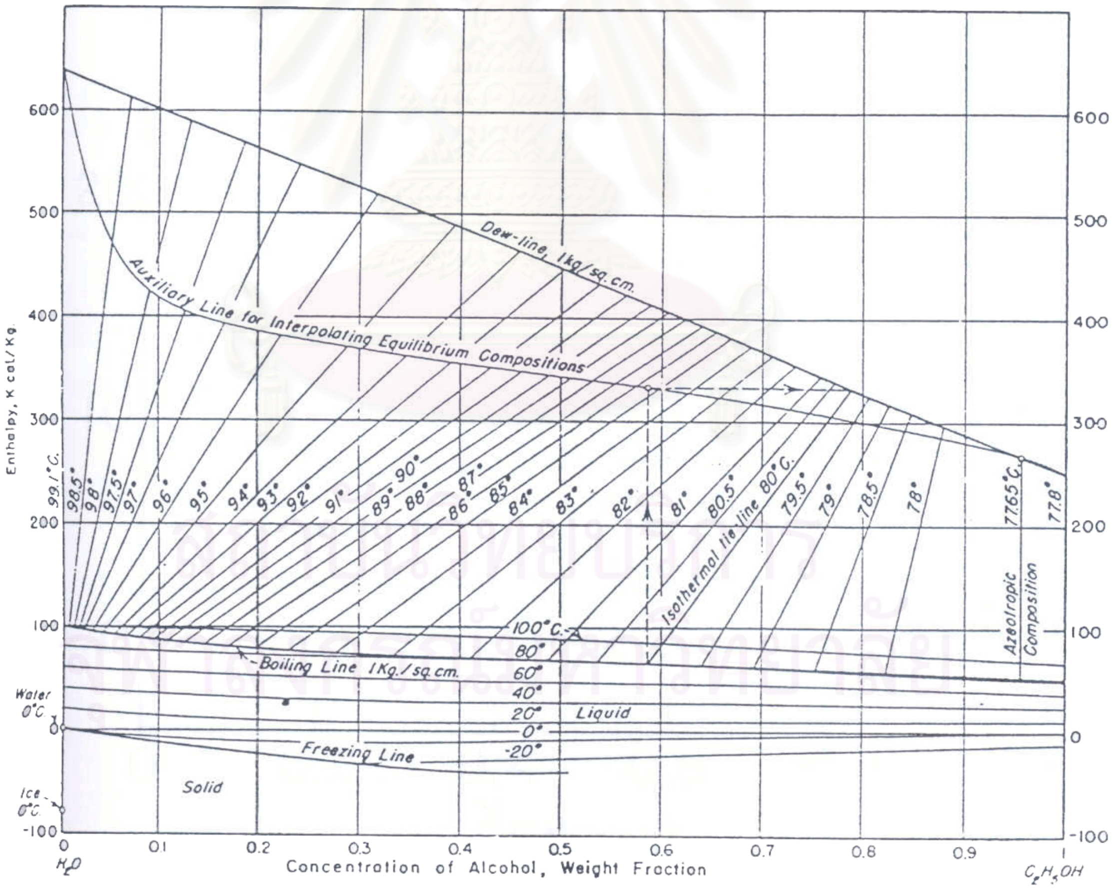


Figure 4.1 Enthalpy-concentration diagram for ethanol(1)+water(2) at 1.013 bar.[14]

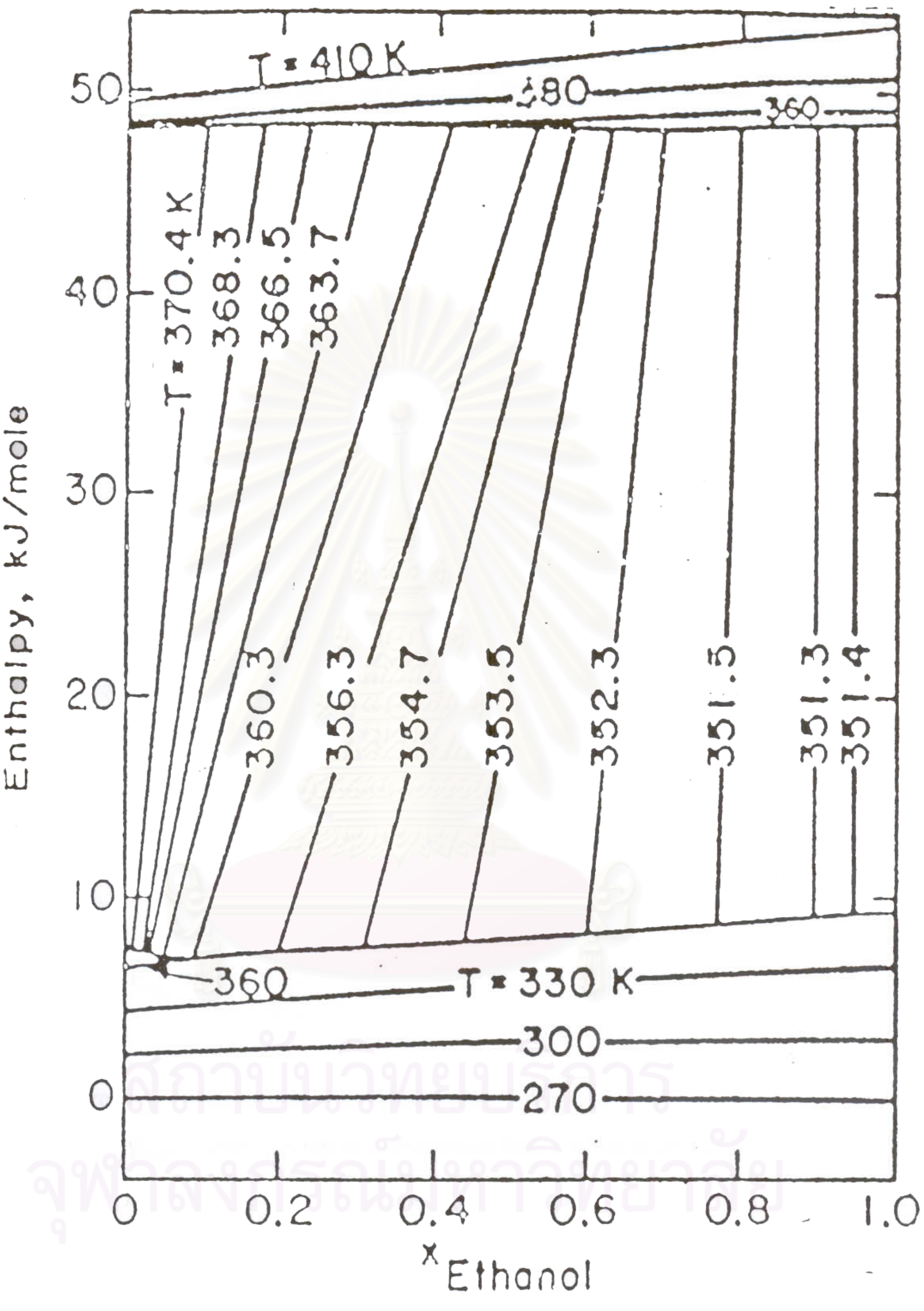


Figure4.2 Enthalpy-concentration diagram for aqueous ethyl alcohol.[16]

4.1.3 Distillation Data

The distillation data of the ethanol/water system determined by Halmu (1976) at Helsinki University of Technology [4] were used as reference in this work. The pilot plant column had 12 sieve plates and 250 mm inside diameter. The column was operated at atmospheric pressure. Table4.5 is shown the configurational data of the distillation column. Table4.6 and Table4.7 are shown one set of actual operating data.

Table4.5 Plate details for the ethanol/water distillation column.[7]

Column diameter	250 mm	Plate spacing	300 mm
Liquid flow path width	233 mm	Hole diameter	2.50 mm
Liquid flow path length	166 mm	Total hole area	0.00579 m^2
Downcomer area	0.00208 m^2	Weir height	40 mm
Active area	0.0449 m^2	Plate thickness	3 mm

In Table4.7, plate efficiency data are computed from the Murphree plate efficiency [7]. The Murphree plate efficiency is defined by comparing a real plate and a theoretical plate. The Murphree vapor phase efficiency is the ratio of actual change between outlet and inlet vapor composition of a real plate to the change of theoretical plate. The Murphree plate efficiency can be expressed also for the liquid phase, but the Murphree vapor phase plate efficiency is more common. The Murphree vapor phase plate efficiency is defined as follows:

$$E_{mv} = \frac{\bar{y}_n - \bar{y}_{n+1}}{y_n^* - \bar{y}_{n+1}} \tag{4-2}$$

where E_{mv} Murphree vapor phase plate efficiency

$\bar{y}_{n+1}$ average vapor composition from the plate below

$\bar{y}_n$ average vapor composition leaving the plate

y_n^* composition of vapor in equilibrium with liquid $\bar{x}_n$ leaving the plate

Table4.6 Distillation operating data.[4]

Feed	Mole fraction of ethanol	$x_F = 0.229$	
	Temperature	$T_F = 82.8$	°C
	Volumetric flow rate	$V_F = 331.1$	l/hr
	Mole fraction flow rate	$F = 196.3$	mol/min
Distillate	Mole fraction of ethanol	$x_D = 0.778$	
	Temperature	$T_D = 74.2$	°C
	Volumetric flow rate	$V_D = 116.5$	l/hr
	Mole fraction flow rate	$D = 37.51$	mol/min
Bottom	Mole fraction of ethanol	$x_B = 0.1034$	
	Temperature	$T_B = 86.0$	°C
	Volumetric flow rate	$V_B = 215.7$	l/hr
	Mole fraction flow rate	$B = 158.8$	mol/min
Reflux	Temperature	$T_R = 78.8$	°C
	Volumetric flow rate	$V_R = 201.0$	l/hr
	Mole fraction flow rate	$R = 64.72$	mol/min
	Reflux Ratio	$r = 1.726$	
Overall mass balance	$F - D - B$	$= \Delta$	Deviation %
(mol/min)	196.3 37.51 158.8	= -0.01	-0.01
Ethanol mole balance	$X_F F - X_D D - X_B B$	$= \Delta$	Deviation %
(mol/min)	44.93 29.18 16.42	= -0.67	-1.5

Table4.7 Distillation liquid composition and temperature data of ethanol(1)+water(2).[4]

Plate	Plate efficiency	x_1	T (^{o}C)
1	1.106	0.755	79.4
2	0.542	0.736	79.6
3	0.610	0.715	80.1
4	0.660	0.690	80.4
5	0.862	0.662	80.1
6	0.545	0.620	80.3
7	0.769	0.591	80.6
8	0.878	0.540	81.2
9	0.735	0.462	81.8
(Feed)10	0.698	0.283	82.9
11	0.573	0.264	84.0
12	0.478	0.263	84.0

4.2 Property Models Used in This Work

4.2.1 Fugacity Coefficient Model

In this work the fugacity coefficient model[15] has been calculated from the virial equation of state. The fugacity coefficient is given by

$$\ln \hat{\phi}_i = \left[2\sum_{j}^{m} y_j B_{ij} - B_{mixture} \right] \frac{P}{RT} \qquad (3\text{-}18)$$

where B_{ij} = second virial coefficient ($i \neq j$)

For binary mixture,

$$B_{mixture} = y_1^2 B_{11} + 2y_1 y_2 B_{12} + y_2^2 B_{22} \qquad (3\text{-}14)$$

4.2.2 Activity Coefficient Model

The Wilson equation was used in this work. The Wilson parameters are calculation from Eqs. (4-3) – Eqs.(4-6).

Wilson equation :

$$\ln\gamma_1 = -\ln(x_1 + A_{12}x_2) + x_2\left[\frac{A_{12}}{x_1 + A_{12}x_2} - \frac{A_{21}}{A_{21}x_1 + x_2}\right] \qquad (3-27)$$

$$\ln\gamma_2 = -\ln(x_2 + A_{21}x_1) - x_1\left[\frac{A_{12}}{x_1 + A_{12}x_2} - \frac{A_{21}}{A_{21}x_1 + x_2}\right] \qquad (3-28)$$

where A_{12} , A_{21} = parameters

Wilson parameters of ethanol(1)+water(2) system are presented in Table4.8.

Table4.8 Data of Wilson parameters for ethanol(1)+water(2) system.[20]

Temperature (K)	Wilson parameter					
	A_{12}	A_{21}	λ_{12}/R	λ_{21}/R	λ_{12}	λ_{21}
303.15	0.23896	0.78925	77.198	428.5	641.864	3562.77
323.15	0.19486	0.83185	148.22	439.78	1232.38	3656.56
343.15	0.17273	0.86504	198.76	453.57	1652.59	3771.21
363.15	0.15985	0.90524	238.49	463.51	1982.93	3853.86

where gas constant R = 8.31451 $J.cm^3$ / mol . K

The relation of Wilson parameters & Temperature are shown in Figure4.3, Figure4.4, Figure4.5 and Figure4.6. The relation of Wilson parameters of ethanol(1)+water(2) with temperature are :

From graphs, linear relation give :

A_{12} = -0.00087525(T) + 0.477 (4-3)

A_{21} = 0.001933167(T) + 0.2035 (4-4)

λ_{12} = 18.736775(T) – 4822.41184 (4-5)

λ_{21} = 4.8515167(T) + 2092.0307 (4-6)

where T is temperature in Kelvin (K).

These equations are used to calculate Wilson parameters in the distillation simulation program. There are many methods to calculation the Wilson parameters. In AppendixC is presented a computer program[12] for calculation Wilson parameters.

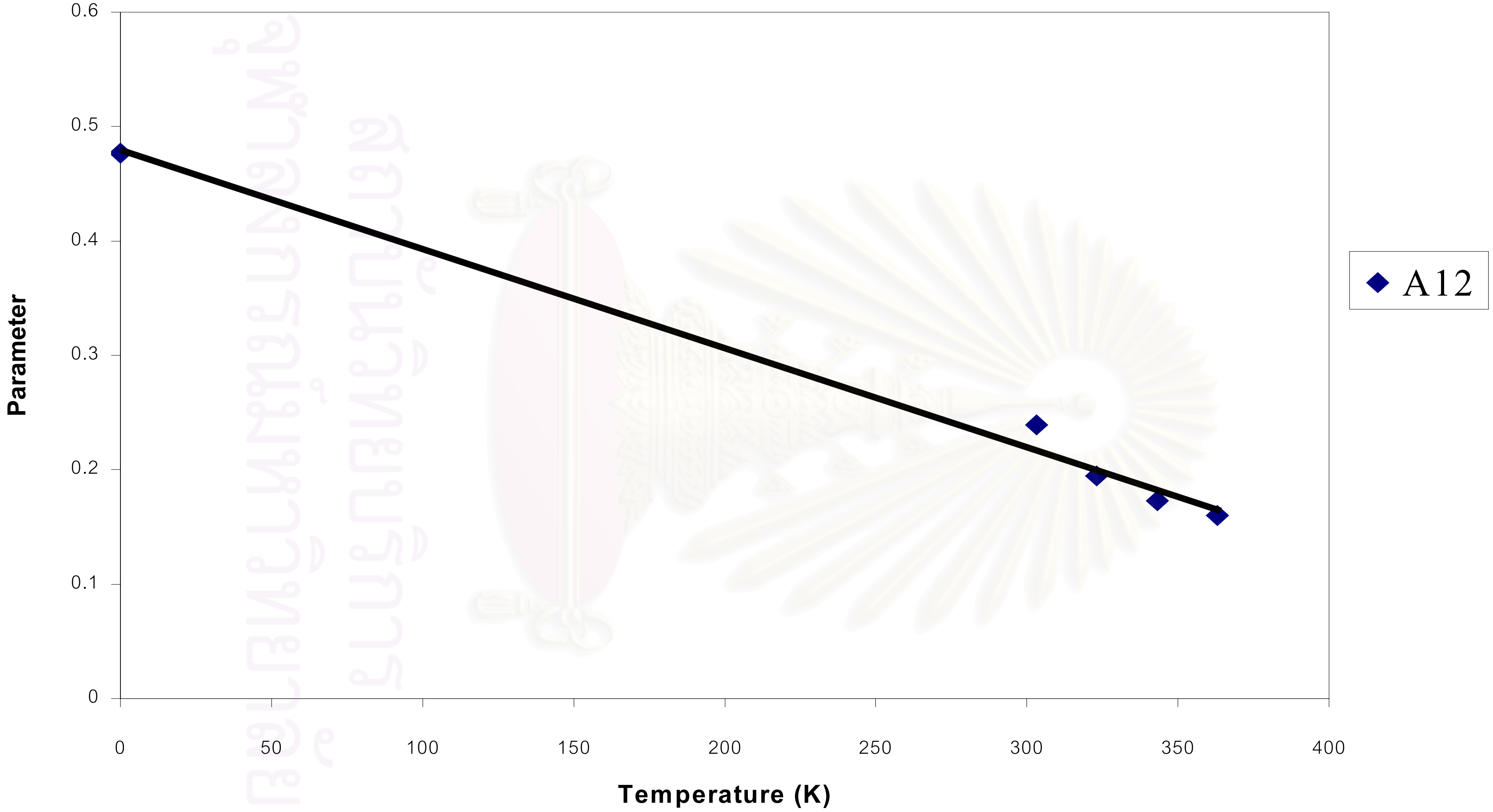


Figure4.3 Wilson parameter (A12) of ethanol(1)+water(2).

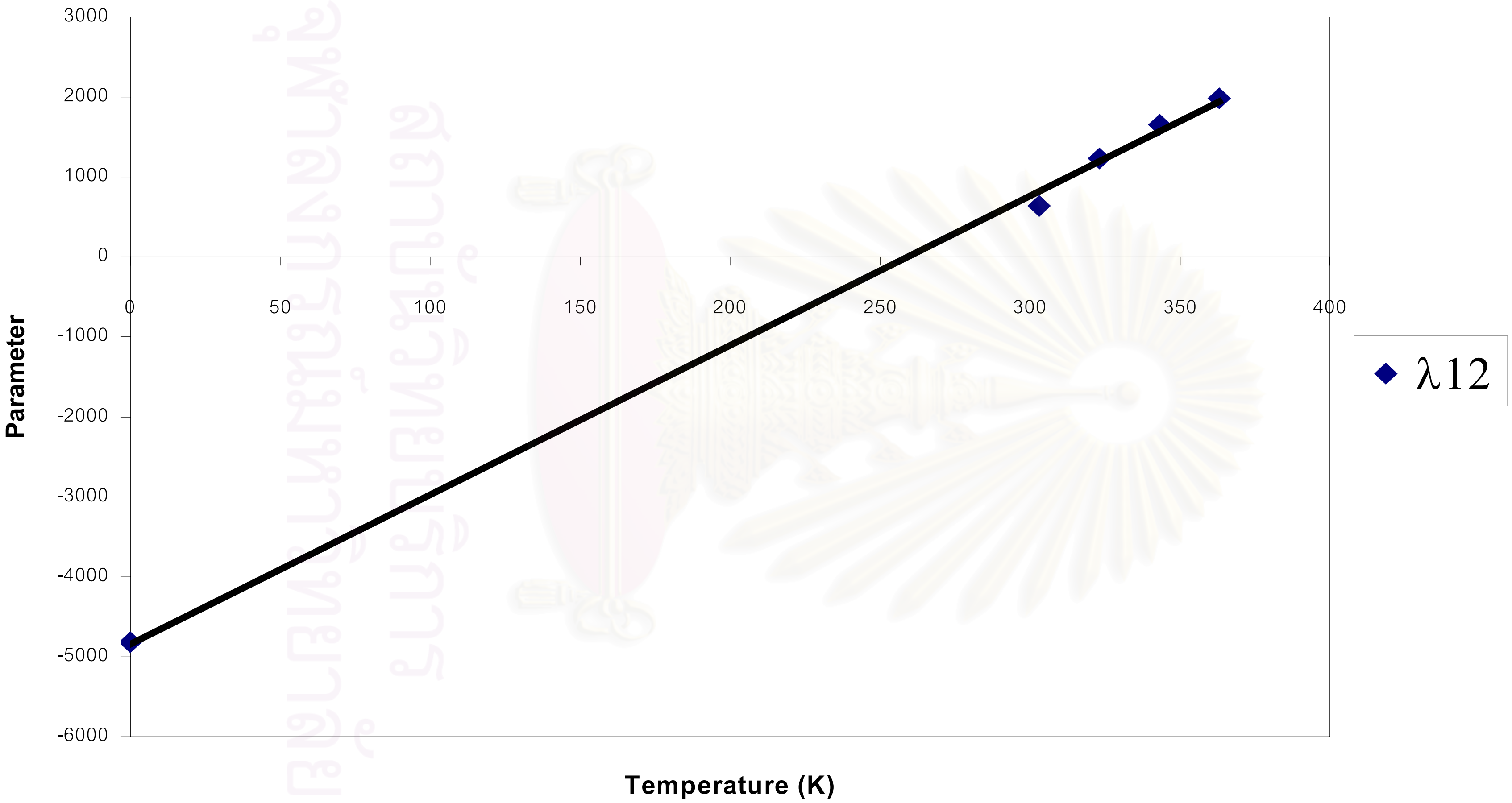


Figure4.4 Wilson parameter (A21) of ethanol(1)+water(2).

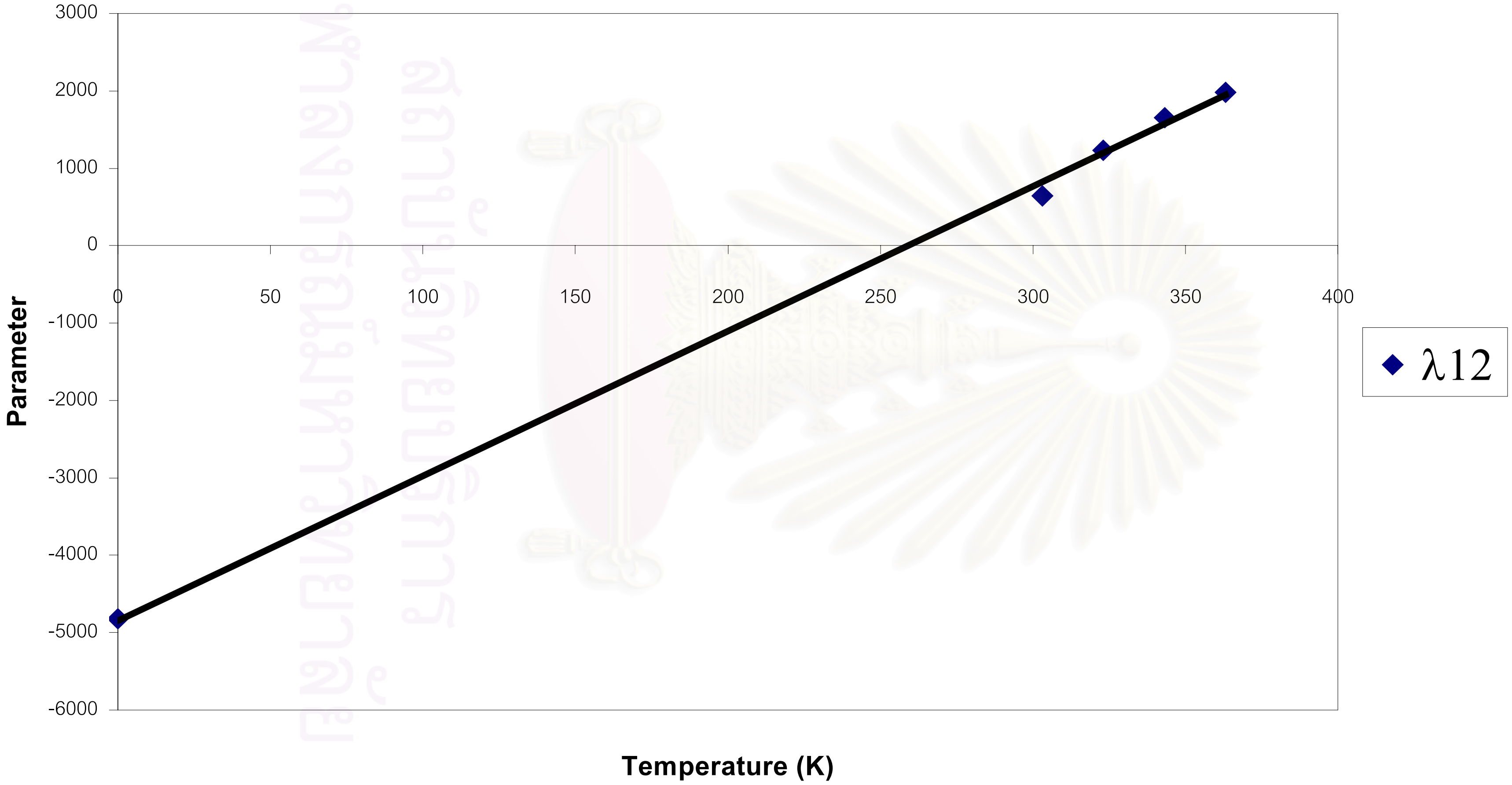


Figure4.5 Wilson parameter (λ12) of ethanol(1)+water(2).

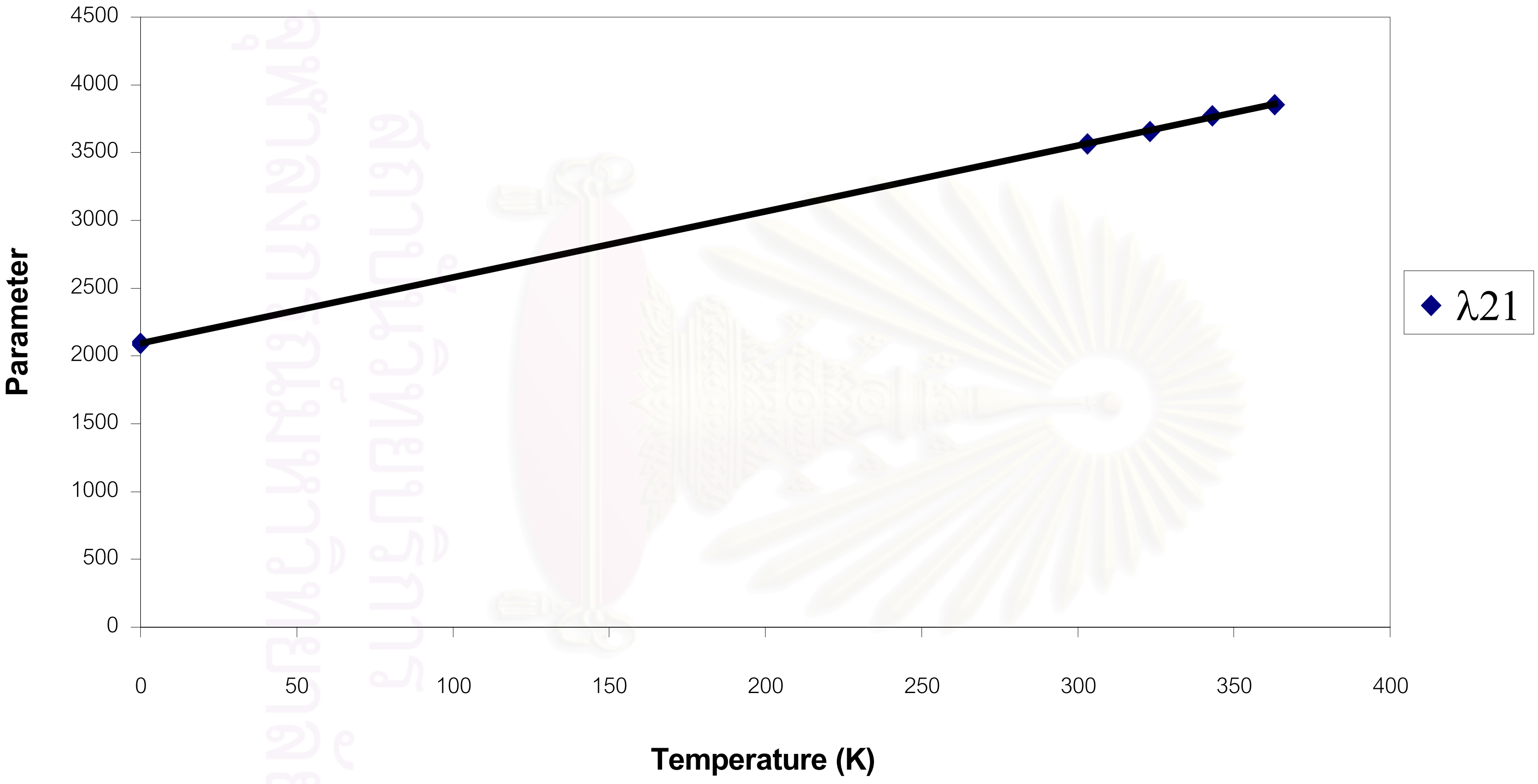


Figure4.6 Wilson parameter (λ21) of ethanol(1)+water(2).

4.2.3 Enthalpy Model

The enthalpy (H_v) model [16] of real vapor mixture is:

$$H_v = \sum_{i=1}^{m} y_i [D_{1i}(T - T_0) + D_{2i} \ln(T/T_0) + D_{3i}(T^2 - T_0^2)/2 + D_{4i}(T\ln T - T_0 \ln T_0 + T_0 - T)]$$

$$-R\sum_{i=1}^{m} T_{ci} P_{ri} [-(0.1445 + 0.073\omega_i) + (0.660 - 0.92\omega_i)/T_{ri} + (0.4155 + 1.50\omega_i)/T_{ri}^2$$

$$+(0.0484 + 0.388\omega_i)/T_{ri}^3 + 0.0657\omega_i/T_{ri}^8] - \sum_{i=1}^{m} x_i \Delta H_{vi} - H_L \qquad (3\text{-}100)$$

where D_{ij} , ω_i= constants of each component

For the latent heat or heat of vaporization of component i (ΔH_{vi})[1] can be calculated from slope of graph of $\ln P^{sat}$ & T. The latent heat (ΔH_{vi}) is the slope of graph multiply by gas constant (R).

$$\Delta H_{vi} = (\text{slope of graph } \ln P^{sat} \text{ \& T}) \text{ x R} \qquad (3\text{-}98)$$

where R=8.31451 J/mol-K.

Figure4.7 and Figure4.8 are shown the slope of graph $\ln P^{sat}$ & T. For ethanol slope of graph $\ln P^{sat}$ & T is -4300 and for water slope is -4400 . Substitution these slope values in equation (3-98) will give the latent heat of ethanol and water. Then the enthalpy of phase change for mixture is :

$$H^{sat,liq} - H^{sat,vap} = -\sum_{i=1}^{m} x_i \Delta H_{vi}$$

For the enthalpy (H_L) model[16] of liquid mixture is:

$$H_L = \sum_{i=1}^{m} x_i [D_{1i}(T - T_0) + D_{2i} \ln(T/T_0) + D_{3i}(T^2 - T_0^2)/2 + D_{4i}(T\ln T - T_0 \ln T_0 + T_0 - T)]$$

$$-R\sum_{i=1}^{m} x_i (-C_{2i} + C_{3i}T^2 + C_{4i}T + 2C_{5i}T^3) + H^E - H_{L,ref} \qquad (3\text{-}110)$$

where D_{ij} , C_{ij} = constants of each component

The excess enthalpy (H^E) can be calculated by the Wilson equation, for binary system the excess enthalpy[20] is:

$$H^E = x_1 x_2 \left(\frac{\lambda_{12} A_{12}}{x_1 + A_{12} x_2} + \frac{\lambda_{21} A_{21}}{A_{21} x_1 + x_2} \right) \qquad (3\text{-}108)$$

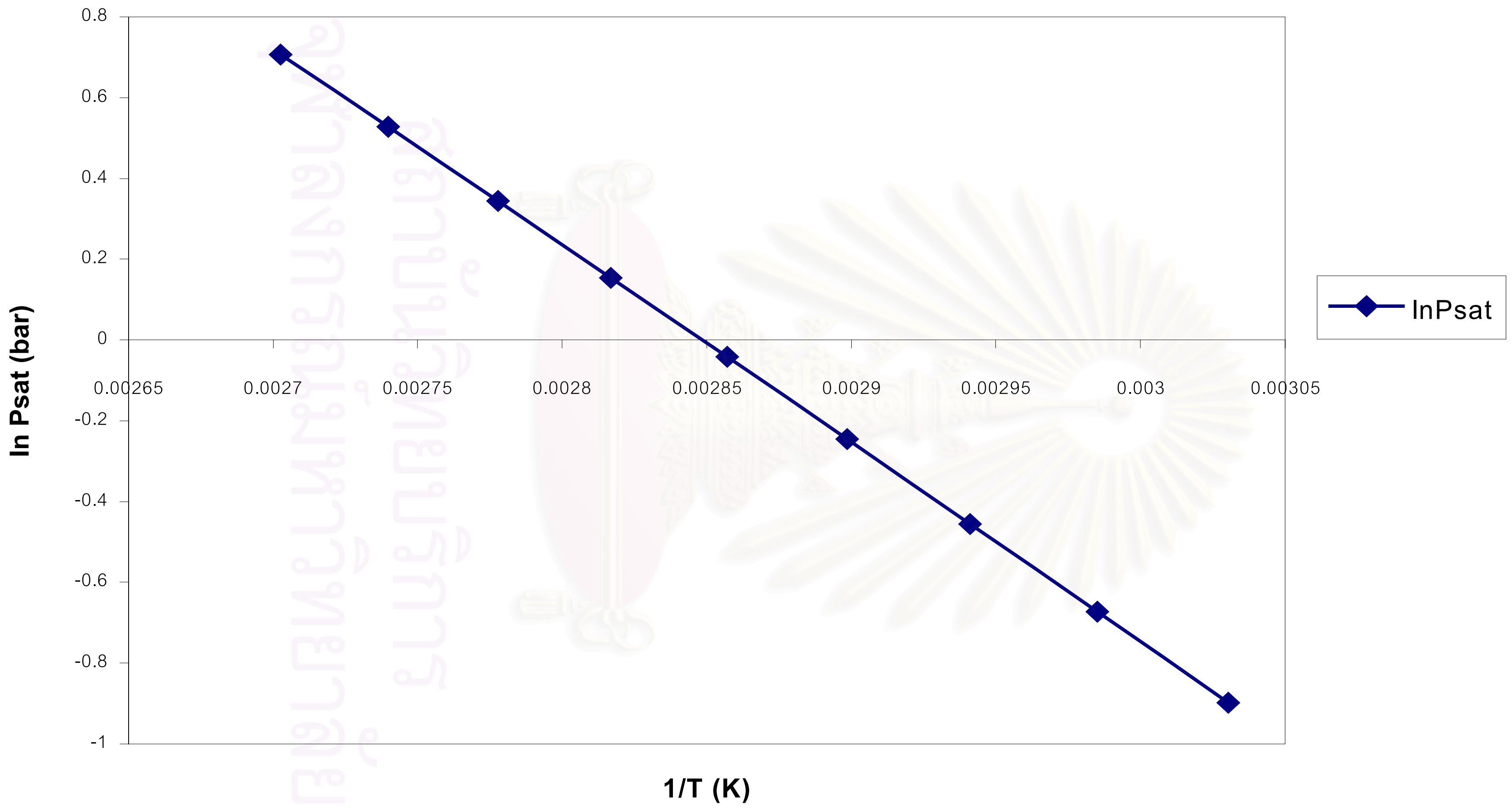


Figure4.7 Relation In Psat & 1/T of ethanol.

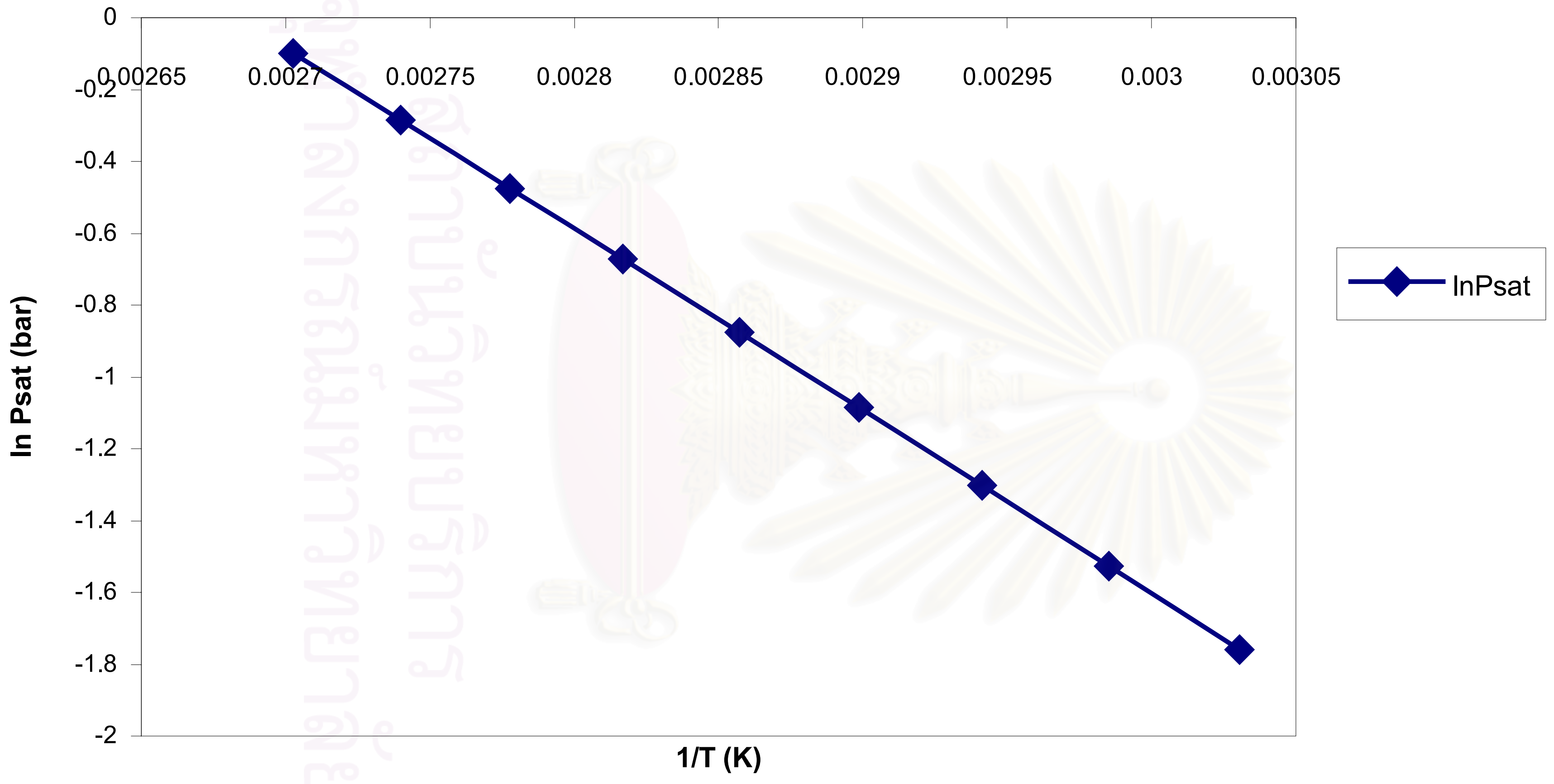


Figure4.8 Relation ln Psat & 1/T of water.

4.2.4 Vapor Pressure Model

The Wagner's vapor pressure model[19] was used in this work.

Wagner equation:

$$\ln\left(\frac{P_{vp}}{P_c}\right) = (1-\tau)^{-1}\left[A\tau + B\tau^{1.5} + C\tau^{3} + D\tau^{6}\right] \qquad (3\text{-}129)$$

where $\tau = 1 - T_r$

P_{vp} = vapor pressure (bar)

T_r = T/T_c = reduced temperature (K)

T_c = critical temperature (K)

A, B, C, D = constants

4.3 Simulation Program

4.3.1 The Model

Tridiagonal Matrix Method [21] is used in this work. Product distribution for multicomponent distillation in complex columns can be computed by this tridiagonal matrix algorithm. The method is simple, fast, and numerically stable. This method is developed for solving problems of multicomponent distillation in complex columns. This method is complies the tridiagonal matrix algorithm for the solutions of the linearized material balance equations, and uses Newton-Ralphson's method for the convergence of column temperature profile. The material balance is solved simultaneously for each component, and therefore no matching is required. Both distributed and non-distributed components are handled with equal ease. The computational procedure is simple, fast, and numerically stable can be readily adapted to digital computers of moderate size.

Mathematical model, the MESH equation, is used in a rigorous equilibrium stage calculation. They are the material balance equation (M), the equilibrium equation (E), the summation equation (S) of mole fractions, and the heat balance equation (H). These four sets of equations are designed as MESH equations that are described in section (2.2) in Chapter 2.

4.3.2 Convergence Method

The Newton-Ralphson's method is used for the convergence of column temperature profile. The problem is to find the value of T that satisfies the equation :

$$f(T) = 0 \tag{4-7}$$

All available numerical methods require a starting estimate of the root, as close as possible to the correct value when there is more than one root.

Steps of Newton-Ralphson's method :

To find a solution to $f(T) = 0$ given the approximation initial value T_0 .

Input : initial value T_0 , tolerance ε , maximum number of iterations N.

Output : approximate solution Z or message of failure.

```
Step1   Set iterative  i = 1.
Step2   While $i \leq N$ do Step3 – Step7.
Step3   Set     $Z = T - f(T) / f'(T)$
Step4   If $|Z - T| < \varepsilon$
            Output (Z);
            Stop.          (procedure completed successfully)
Step5   Set i = i+1.
Step6   Set T = Z
Step7   Output " Method failed after N iterations " ;
            Stop.
```

4.3.3 Computer Flow Chart

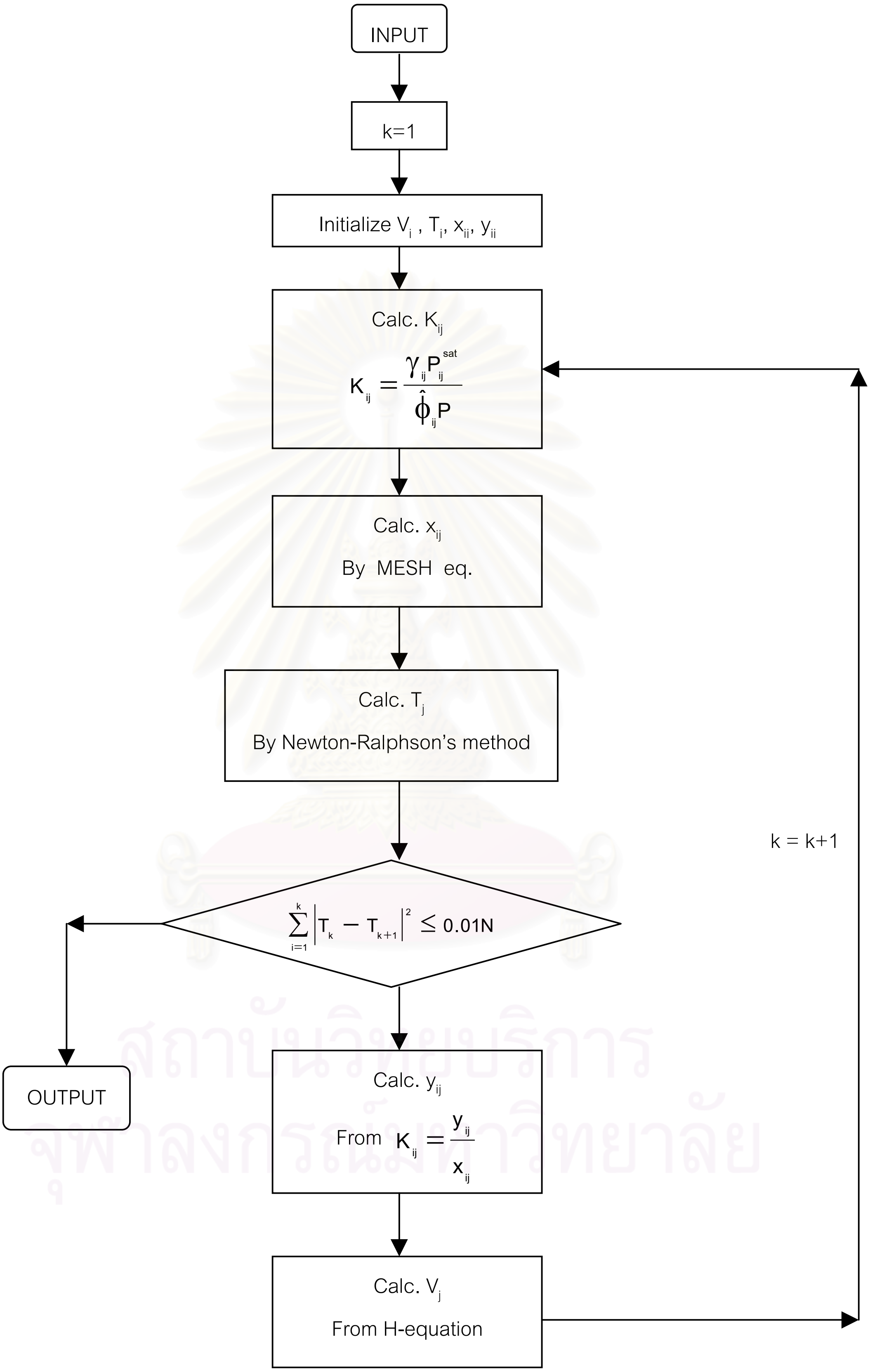


Figure4.9 The computer flow chart.

Method for Calculation Distillation

The method for distillation [14], particularly when the components involved cover a relatively narrow range of volatility, proceeds iterative by the following steps, where k is the iteration index for the entire distillation column.

1. Specify number of stage (N) and all values of $z_{i,j}$, F_j, T_{Fj}, P_{Fj}, P_j, U_j, W_j, and Q_j, except Q_1 and Q_N. For this work is a conventional column all the quantities of the external streams except $z_{i,j}$, F_j, T_{Fj}, P_{Fj}, P_j, B, D, Q_1 and Q_N are zero.

2. Specify type of condenser. If total ($U_1 \neq 0$), compute L_N from overall material balance; if partial ($U_1=0$), specify V_1 and compute L_N from overall material balance. In this case it is total condenser ($U_1 \neq 0$).

3. Specify reflux rate L_1, assuming no subcooling, $L_1= r * D$ (r is reflux ratio).

4. Compute $V_2 = V_1 + L_1 + U_1 - F_1$. For this case $F_1=0$ (no feed in stage 1), $V_1=0$ (no vapor out from stage 1, total condenser) and $U_1=D$ (from $V_1=U_1+D$ when $V_1=0$). Give $V_2 = L_1 + D$.

5. Provide initial guesses (k=0) or values of all tear variables T_j and V_j($j>2$). Temperature guesses are readily obtained by linear interpolation between estimates of top and bottom-stage temperatures. The bottom-stage temperature is estimated by making a bubble-point-temperature calculation by using an estimate of distillate composition; otherwise, for a partial condenser, a dew-point temperature calculation is made. An estimate of the vapor-rate profile is readily obtained by assuming constant molar overflow down the column.

6. Set index k=1 to initiate the first column iteration.

7. Using specified stage pressures, current estimates of stage temperatures, and current estimates of stage vapor-and liquid-phase stage compositions estimate all K_{ij} values (for k=1, initial estimates of stage phase compositions may be necessary if $K_{i,j}$ values are sensitive to phase compositions).

8. Compute values of $x_{i,j}$ by solving Eqs. (2-27) through (2-28) by the tridiagonal-matrix algorithm once for each component. Unless all mesh equations are converged, $\sum x_{i,j} \neq 1$ for each stage j.

9. To force $\sum x_{i,j}=1$ at each stage j, normalize values by the replacement $x_{i,j}=x_{i,j}/\sum x_{i,j}$

10. Compute a new set of values of $T_j^{(k)}$ tear variables by computing, one at a time, the bubble-point temperature at each stage based on the specified stage pressure and corresponding normalized and Eq.(2-11) to eliminate $y_{i,j}$ to give

$$\sum_{i=1}^{m} K_{ij} x_{ij} - 1 = 0 \tag{2-24}$$

which is a nonlinear equation in $T_j^{(k)}$ and must be solved iteratively by some appropriate root-finding method, such as the Newton-Ralphson or the Muller method.

11. Compute values of $y_{i,j}$ once at a time from Eq. (2-10)

12. Compute a new set of values of the V_j tear variables one at a time, starting with V_3, from an energy-balance equation that is obtained by combining Eqs. (2-12) and (2-18), eliminating L_{j-1} and L_f to give

$$V_j = (C_{j-1} - A_{j-1}V_{j-1}) / B_{j-1} \tag{4-8}$$

where

$$A_{j-1} = H_{Lj-2} - H_{Vj-1}$$

$$B_{j-1} = H_{Vj} - H_{Lj-1}$$

$$C_{j-1} = \left[\sum_{m=1}^{j-2}(F_m - W_m - U_m) - V_1\right](H_{Lj-1} - H_{Lj-2}) + F_{j-1}(H_{Lj-1} - H_{Fj-1})$$
$$+ W_{j-1}(H_{Vj-1} - H_{Lj-1}) + Q_{j-1}$$

13. Check to determine if the new sets of tear variables $T_j^{(k)}$ and $V_j^{(k)}$ are within some prescribed tolerance of sets $T_j^{(k-1)}$ and $V_j^{(k-1)}$ used to initiate the current column iteration. A possible convergence criterion is

$$\sum_{j=1}^{N}\left[\frac{T_j^{(k)} - T_j^{(k-1)}}{T_j^{(k)}}\right]^2 + \sum_{j=3}^{N}\left[\frac{V_j^{(k)} - V_j^{(k-1)}}{V_j^{(k)}}\right]^2 \le 10^{-7} N \tag{4-9}$$

but Wang and Henke [21] use

$$\sum_{j=1}^{N}\left[T_j^{(k)} - T_j^{(k-1)}\right]^2 \le 0.01N \qquad (N = \text{number of stages}) \tag{4-10}$$

14. If the convergence criterion is met, compute values of L_j from Eq. (2-13) and values of Q_1 and Q_N from Eq. (2-12). Otherwise, set k = k+1 and repeat steps 7 to 14.

Step 14 implied that if the calculations are not converged, values of $T_j^{(k)}$ computed in step 10 and values of $V_j^{(k)}$ computed in step 12 are used as values of the tear variables to initiate iteration k+1. This is the method of successive substitution, which may require a large number of iterations and/or may result in oscillation. Alternatively, values of $T_j^{(k)}$ and $V_j^{(k)}$ can be adjusted prior to initiating iteration k+1. Experience indicates that values of T_j should be reset if they tend to move outside of specified upper and lower bounds and that negative V_j values be reset to small positive values. Also, damping can be employed to prevent values of absolute T_j and V_j from changing by more than, say, 10 percent of successive iterations.

4.3.4 Variables Studied

In distillation simulation, the thermodynamic property models are needed. From Chapter 3, equation (3-8) :

$$K_i = \frac{y_i}{x_i} = \frac{\gamma_i f_i}{\hat{\phi}_i P} = \frac{\gamma_i P_i^{sat}}{\hat{\phi}_i P}$$

The necessary thermodynamic property models in distillation simulation are : activity coefficient (γ_i) model, saturated(vapor) pressure (P^{sat}) model and fugacity coefficient ($\hat{\phi}_i$) model. The distillation simulation depends on these property models. To study the effect of inaccuracy of the thermodynamic property models on distillation simulation, it is necessary to study these properties. These properties are related to the vapor-liquid equilibrium constant (K-value) as shown in Eq.(3-8). Normally, the saturated pressure (P^{sat}) and the fugcity coefficient ($\hat{\phi}_i$) are quite accurate. Then the property effect on the vapor-liquid equilibrium constant (K-value) is activity coefficient (γ_i). Moreover, in MESH equation there is additional property that is necessary for distillation simulation. It is enthalpy (H) model.

However, the distillation simulation is also depended on the design condition. The number of stage (N) and reflux ratio (r) are selected to study the effect. Then the variables studied in this work are the activity coefficient (γ_i), the enthalpy (H) model, number of stage (N) and the reflux ratio (r).

CHAPTER 5

RESULTS AND DISCUSSION

5.1 Accuracy of Property Models

5.1.1 Accuracy of Vapor Pressure Model

Wagner’s vapor pressure model is selected in this work. The accuracy of this model can be calculated by computer program in AppendixB. In AppendixG Table5.1 is shown the accuracy of model for ethanol and Table5.2 for water. The experiment data are from Perry’s Chemical Engineers’ Handbook [14]. The saturated pressure of ethanol and water from calculation and experiment are shown in Figure5.1 and Figure5.2. The experiment data is from Perry’s Chemical Engineers’ Handbook [14]. From Table5.1 and Table5.2 % Average Absolute Deviation are 2.56% and 0.12% respectively.

5.1.2 Accuracy of Activity Coefficient Model

The selected activity coefficient model is Wilson equation. The accuracy can be determined by computer program. The accuracy of Wilson’s activity coefficient model for ethanol is shown in Table5.3 and Table5.4 for water. Table5.3 and Table5.4 are in AppendixG.

The activity coefficient of ethanol and water data are shown in Figure5.3 and Figure5.4. From Table5.3 and Table5.4 % Average Absolute Deviation are 1.14% for ethanol and 1.39% for water.

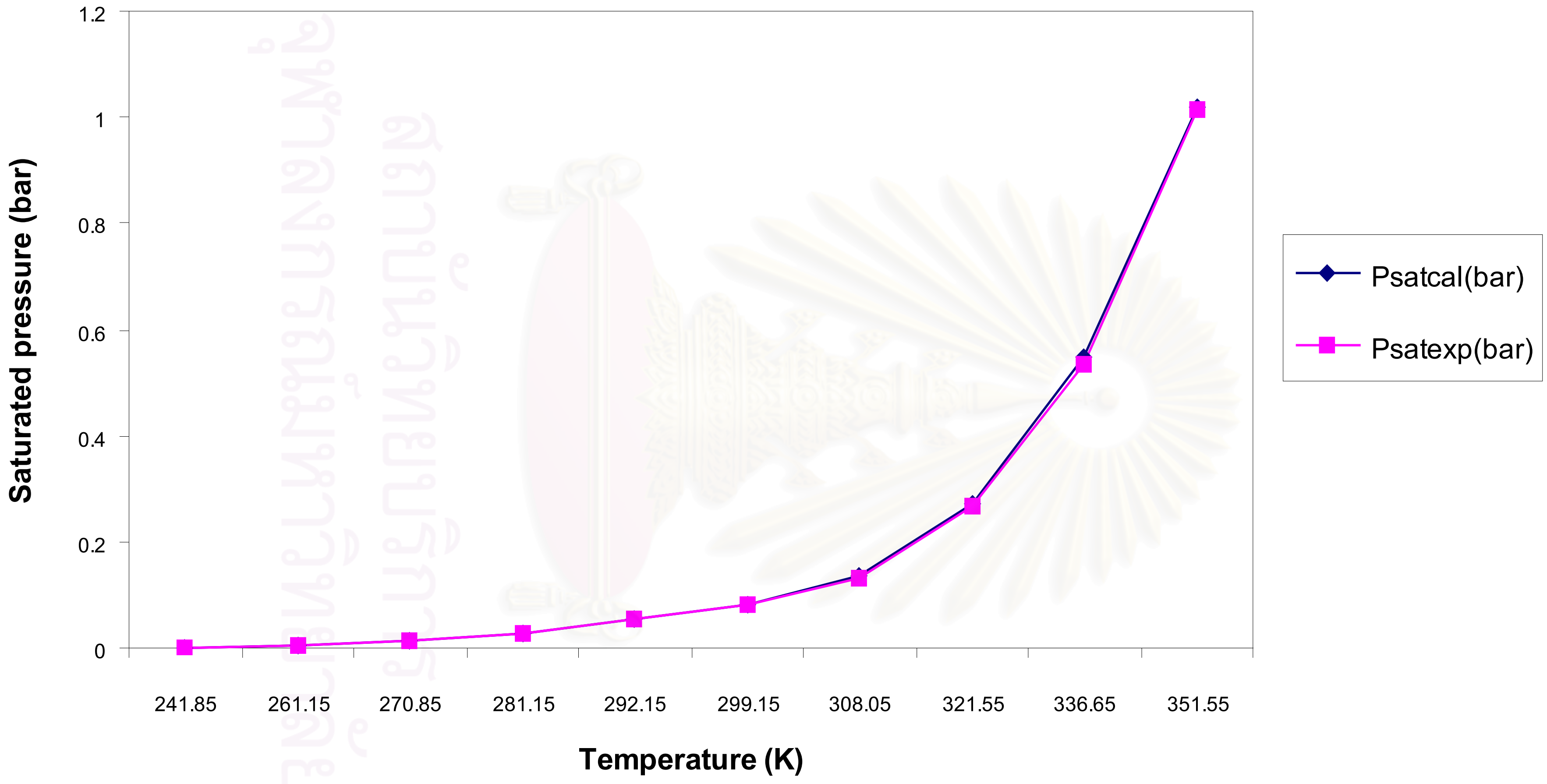


Figure5.1 Saturated pressure of ethanol.

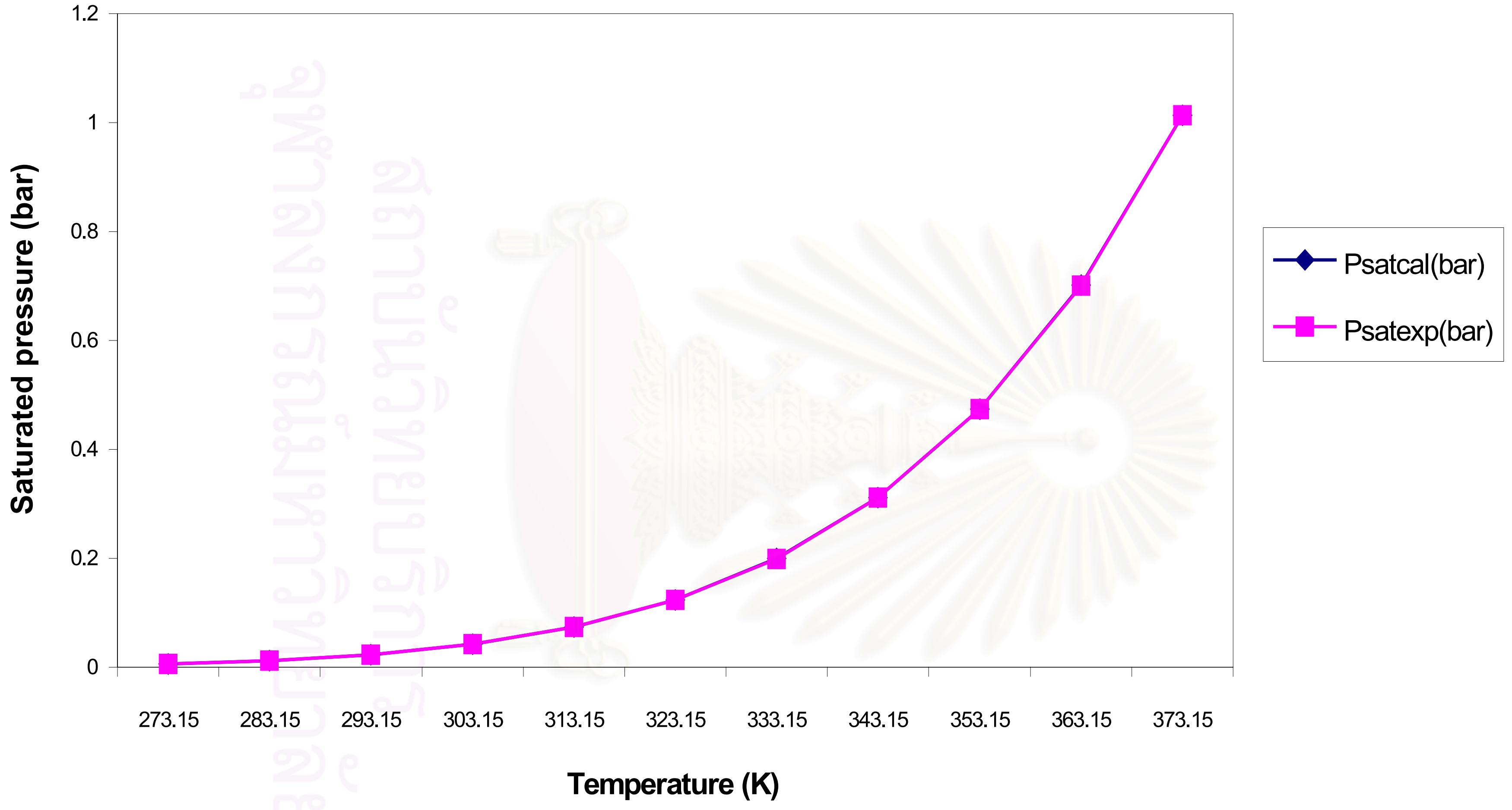


Figure5.2 Saturated pressure of water.

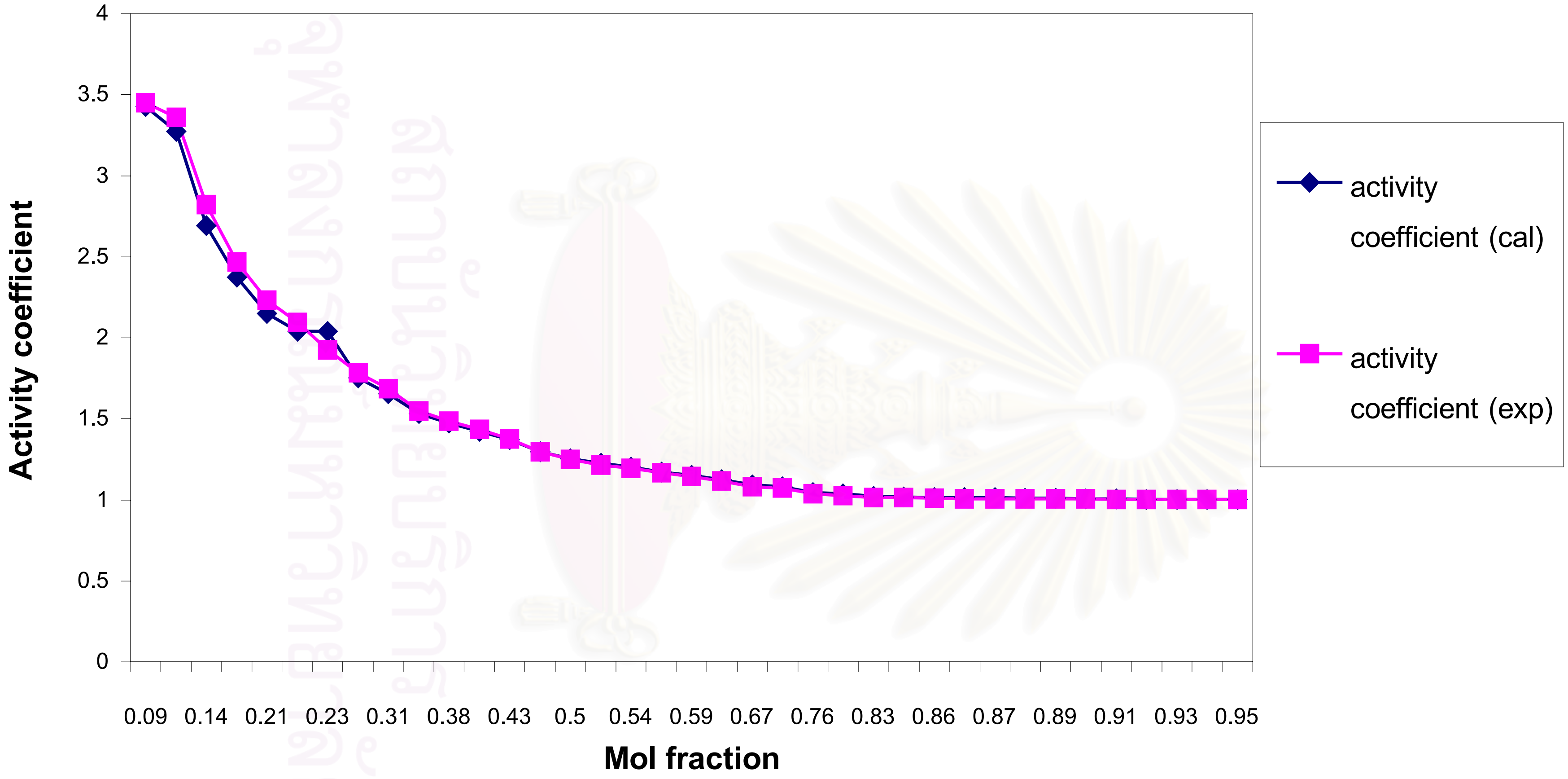


Figure5.3 The activity coefficient of ethanol.

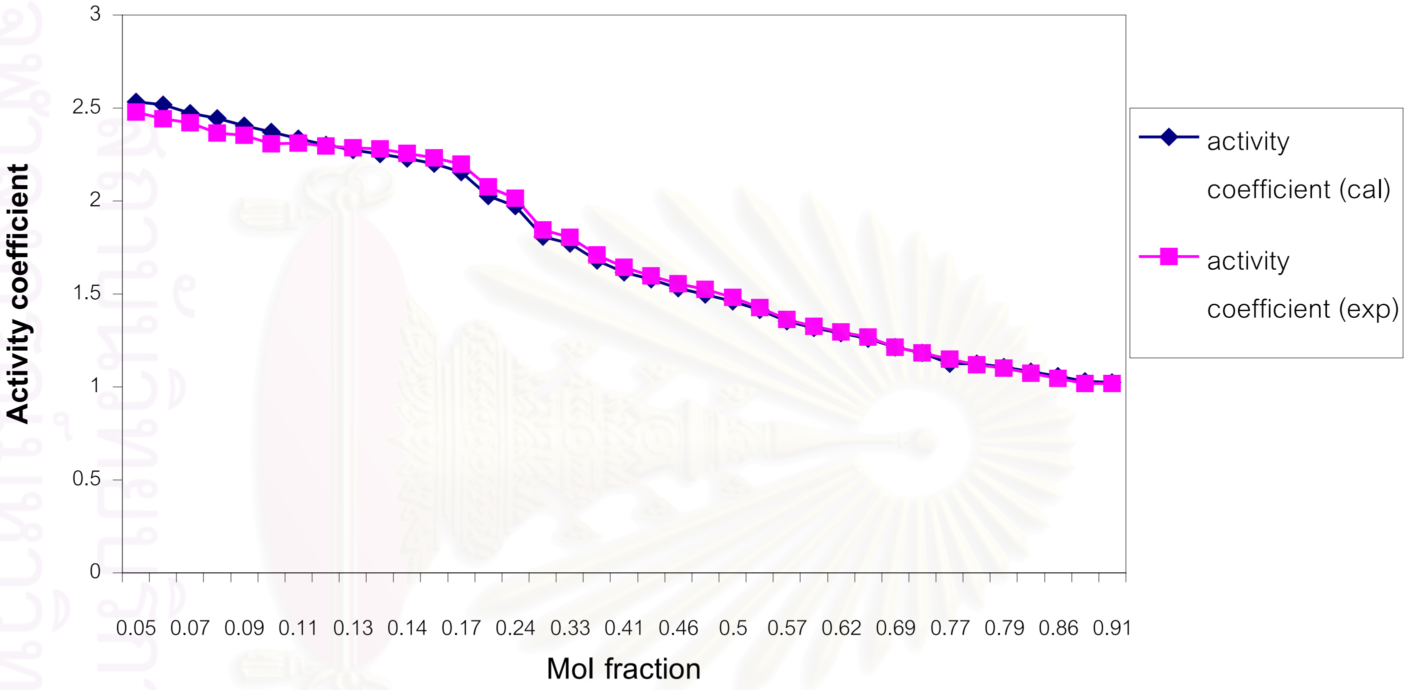


Figure5.4 Activity coefficient of water.

5.1.3 Accuracy of Fugacity Coefficient

The fugacity coefficient was developed using virial coefficient [15]. The fugacity coefficient is given by Eq.(3-18). AppendixE is presented the computer program that developed from Prausnitz,1967 [15]. The average errors in the virial coefficient in this program were less than 10% and 100 cc/gmol. This program was developed using virial coefficients for 50 substances. These include such compound as ethanol and water.

The fugacity coefficient depends on pressure, temperature, and vapor composition; this dependence, in the moderate pressure region as described by truncated virial equation, is usually as follows.

(a) At constant temperature and composition, an increase in pressure almost always causes the fugacity coefficient ($\hat{\phi}_i$) to depart further from unity, usually in the direction $\hat{\phi}_i$ < 1.

(b) At constant pressure and composition, increase in temperature almost always causes $\hat{\phi}_i$ to become nearer to unity.

(c) At constant pressure and temperature, the effect of composition on $\hat{\phi}_i$ is strongest when y_i is small. If y_i is near unity, a change in composition has relatively little effect on $\hat{\phi}_i$. However, it dose not necessarily follow that $\hat{\phi}_i$ comes closer to unity as y_i increase. In fact for a very heavy component i mixed a very light component j, it frequently happens that $\hat{\phi}_i$ is nearer to unity for small y_i than it is for small y_j.

From using this computer program to calculate the fugacity coefficient in this work. Table5.5 is shown the calculation results by using the isobaric VLE data [9].

5.1.4 Accuracy of Enthalpy

The enthalpy of liquid mixture can be calculated from Eq.(3-110). The accuracy can be determined by computer program in AppendixF. The accuracy of enthalpy model for liquid mixture is shown in Table5.6. The enthalpy of vapor mixture can be calculated from Eq.(3-100). The accuracy of enthalpy model for vapor mixture is shown in Table5.7. Table5.6 and Table5.7 are in AppendixG. The enthalpy of liquid and vapor mixture of ethanol(1)+water(2) data are shown in Figure5.5, Figure5.6 and Figure5.7.For the enthalpy of vapor mixture are shown in Figure5.8. From Table5.6 and Table5.7 % Average Absolute Deviation are 2.25% for liquid and 1.65% for vapor mixture.

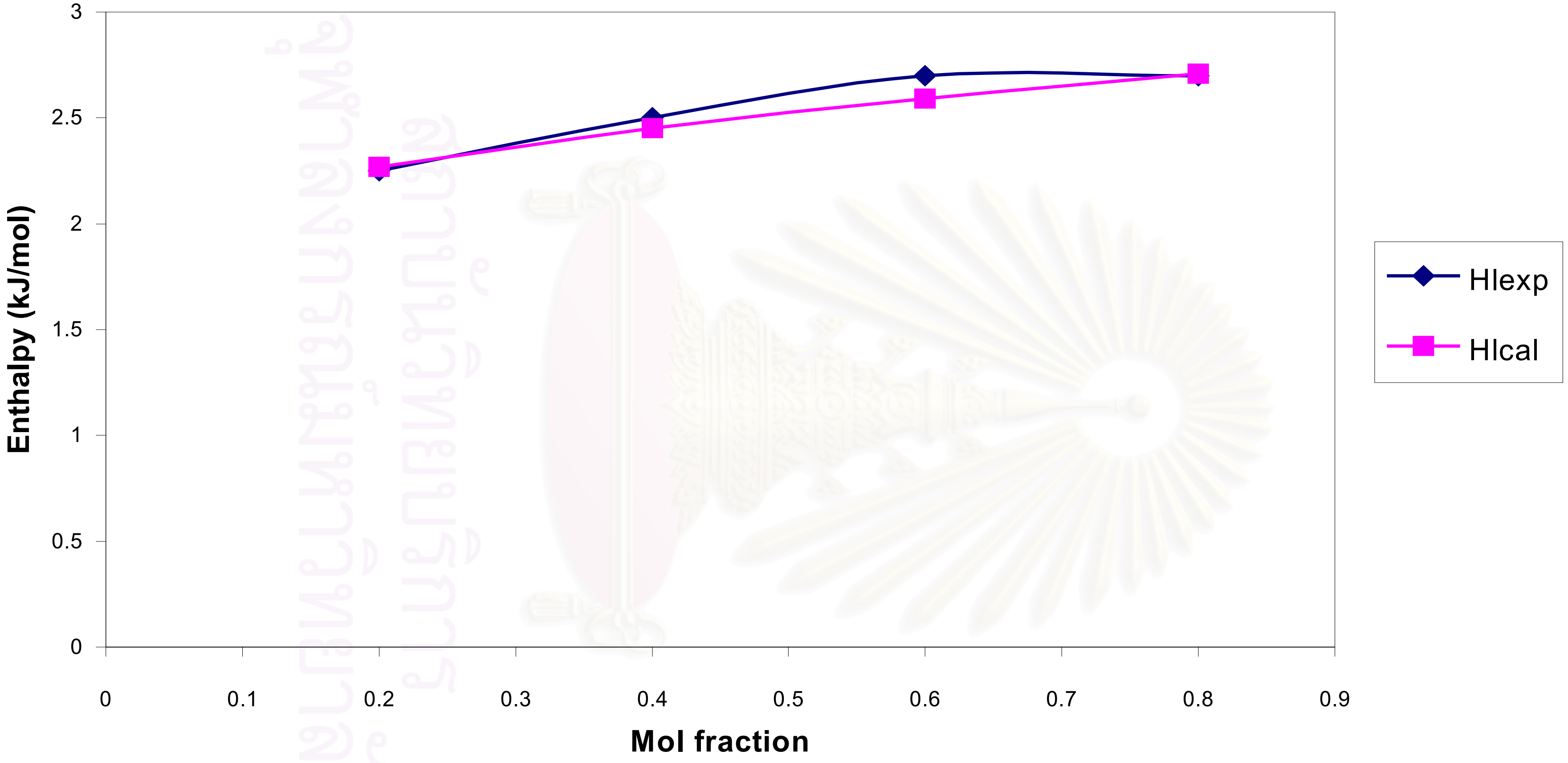


Figure5.5 Enthalpy of liquid phase of ethanol+water at 300K.

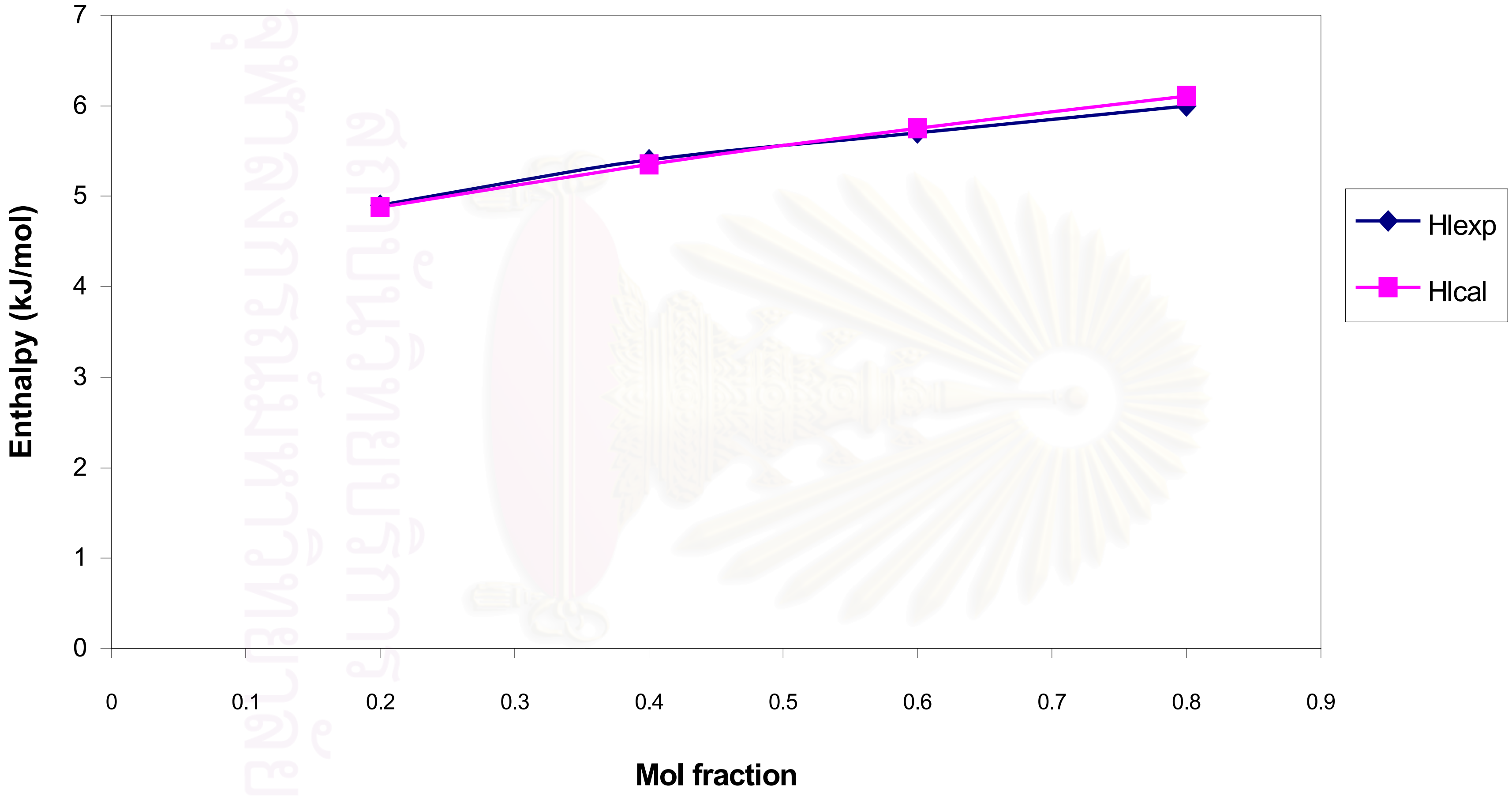


Figure5.6 Enthalpy of liquid phase of ethanol+water at 330K.

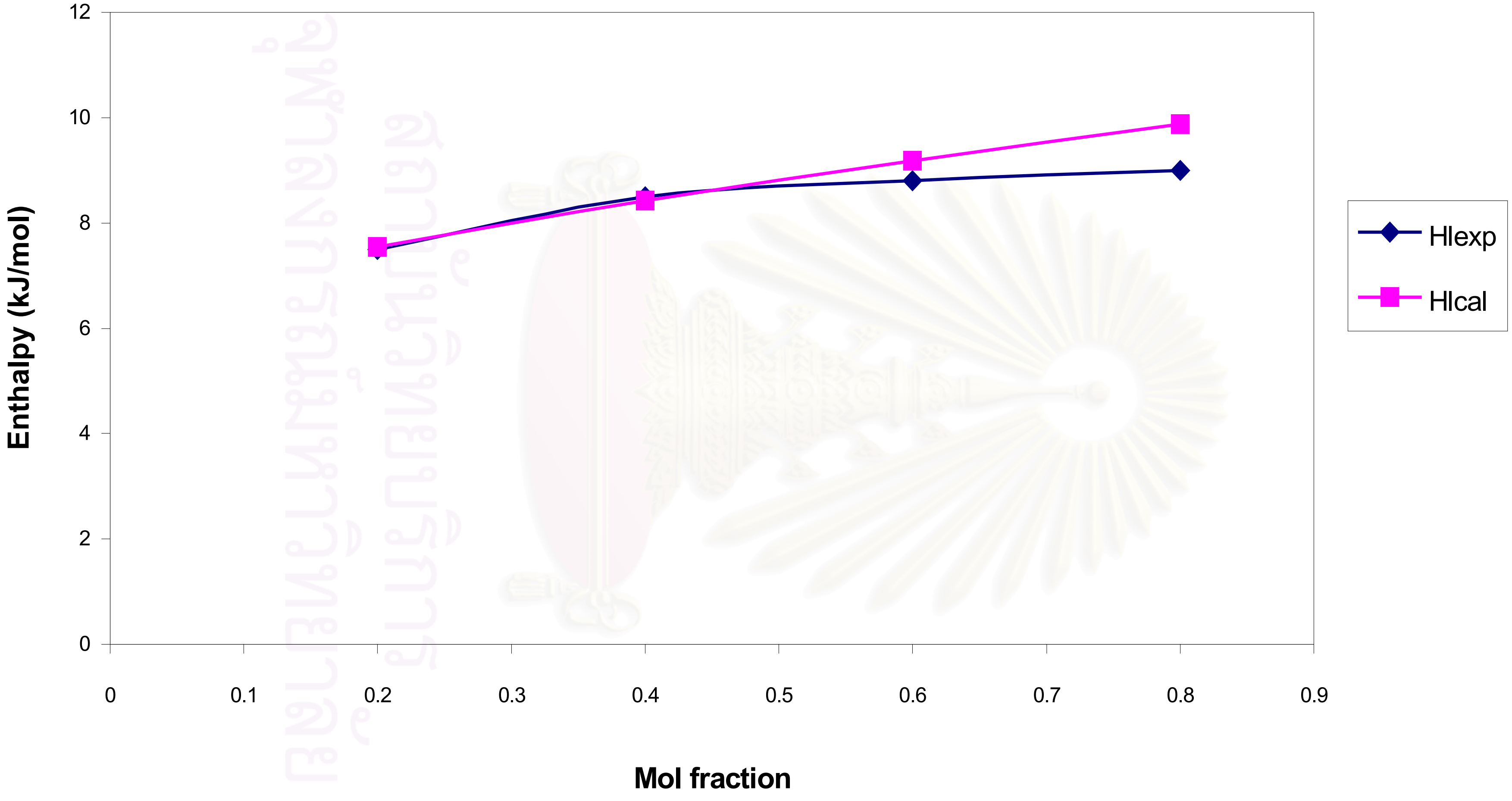


Figure5.7 Enthalpy of liquid phase of ethanol+water at 360K.

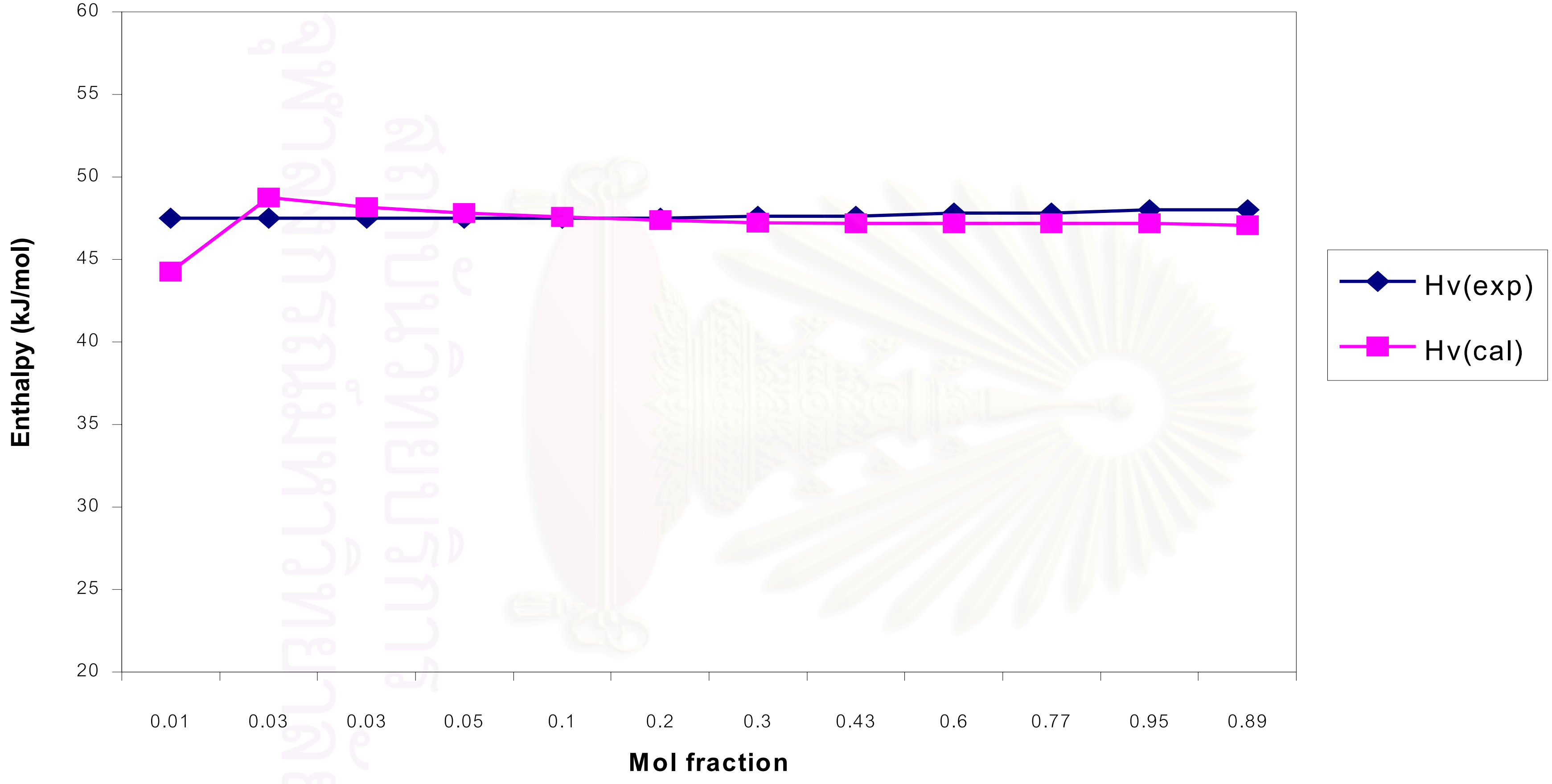


Figure5.8 Enthalpy of vapor phase of ethanol+water.

5.2 Effect of Inaccuracy of Property Model

5.2.1 Effect of Inaccuracy in Activity Coefficient Model on K-value

The selected activity coefficient model is Wilson equation. The accuracy of model depends on the Wilson parameters. The inaccuracy Wilson parameters provide the inaccuracy of model. The inaccuracy at any Wilson parameters at temperature 323.15K are shown in Table5.8 - Table5.35 in AppendixG.

From Table5.8-Table5.35 are shown %Average Absolute Deviation (%AAD) of the inaccuracy property model. The inaccuracy activity coefficient model provide the error properties while the Wilson parameter has high error the properties also have high error. Then the vapor-liquid equilibrium constant (K-value) is also error at same %AAD. The %Average Absolute Deviation of all are presented in Table5.36 and Figure5.9

5.2.2 Effect of Inaccuracy in Enthalpy

The enthalpy of liquid mixture can be calculated from equation (3-110) and the enthalpy of vapor mixture can be calculated from equation (3-100).The accuracy of both models depend on the constants of models. The inaccuracy constants provide the inaccuracy model. The inaccuracy of model at any constant(D_1) are shown in Table5.37 - Table5.56 in AppendixG.

The % Average Absolute Deviation of enthalpy model at any constant(D_1) of model are shown in Figure5.10. The figure show that the %AAD depend on the constant (D_1) of model. From Table5.37-Table5.56 are shown the distillation simulation results at any %Average Absolute Deviation (%AAD) of the inaccuracy property model. The inaccuracy enthalpy model provide the error properties while the constant (D_1) of the model has high error the properties also have high error.

Table5.36 The %Average Absolute Deviation of the vapor-liquid equilibrium constant (K-value) by varying the Wilson parameter.

Wilson parameter (A_{21})	% Average Absolute Deviation (%AAD)
0.10 A_{21}	-127.22
0.20 A_{21}	-97.31
0.30 A_{21}	-75.11
0.40 A_{21}	-57.62
0.50 A_{21}	-43.63
0.55 A_{21}	-37.58
0.60 A_{21}	-32.04
0.65 A_{21}	-26.93
0.70 A_{21}	-22.20
0.75 A_{21}	-17.81
0.80 A_{21}	-13.72
0.85 A_{21}	-9.99
0.90 A_{21}	-6.30
0.95 A_{21}	-3.22
1.05 A_{21}	+4.18
1.10 A_{21}	+6.66
1.15 A_{21}	+9.25
1.20 A_{21}	+11.75
1.25 A_{21}	+14.14
1.30 A_{21}	+16.44
1.35 A_{21}	+18.63
1.40 A_{21}	+20.75
1.45 A_{21}	+22.77
1.50 A_{21}	+24.75
1.60 A_{21}	+28.37
1.70 A_{21}	+31.74
1.80 A_{21}	+34.88
1.90 A_{21}	+37.79

Note: + is deviation when increase Wilson parameter (A_{21})

- is deviation when decrease Wilson parameter (A_{21})

Table5.57 The %Average Absolute Deviation of inaccuracy enthalpy model.

Constant of Enthalpy Model (D_1)	% Average Absolute Deviation (%AAD)
$0.90D_1$	-53.36
$0.91D_1$	-49.05
$0.92D_1$	-44.75
$0.93D_1$	-40.48
$0.94D_1$	-36.34
$0.95D_1$	-33.42
$0.96D_1$	-30.79
$0.97D_1$	-28.05
$0.98D_1$	-25.45
$0.99D_1$	-23.21
$1.01D_1$	+19.30
$1.02D_1$	+18.10
$1.03D_1$	+17.71
$1.04D_1$	+19.43
$1.05D_1$	+23.18
$1.06D_1$	+27.72
$1.07D_1$	+32.99
$1.08D_1$	+37.98
$1.09D_1$	+42.88
$1.10D_1$	+47.84

Note: + is deviation when increase constant (D_1) of the enthalpy model

- is deviation when decrease constant (D_1) of the enthalpy model

5.3 Simulation Results

The simulation results are computed by simulation distillation program in AppendixA with accurate property models. The simulation results of ethanol(1)+water(2) distillation are shown in the Table5.59. These simulation results are agree with the experimental data with only small deviation as shown in Table5.58 and Figure5.11and Figure5.12. Table5.58 and Table5.59 are in AppendixG.

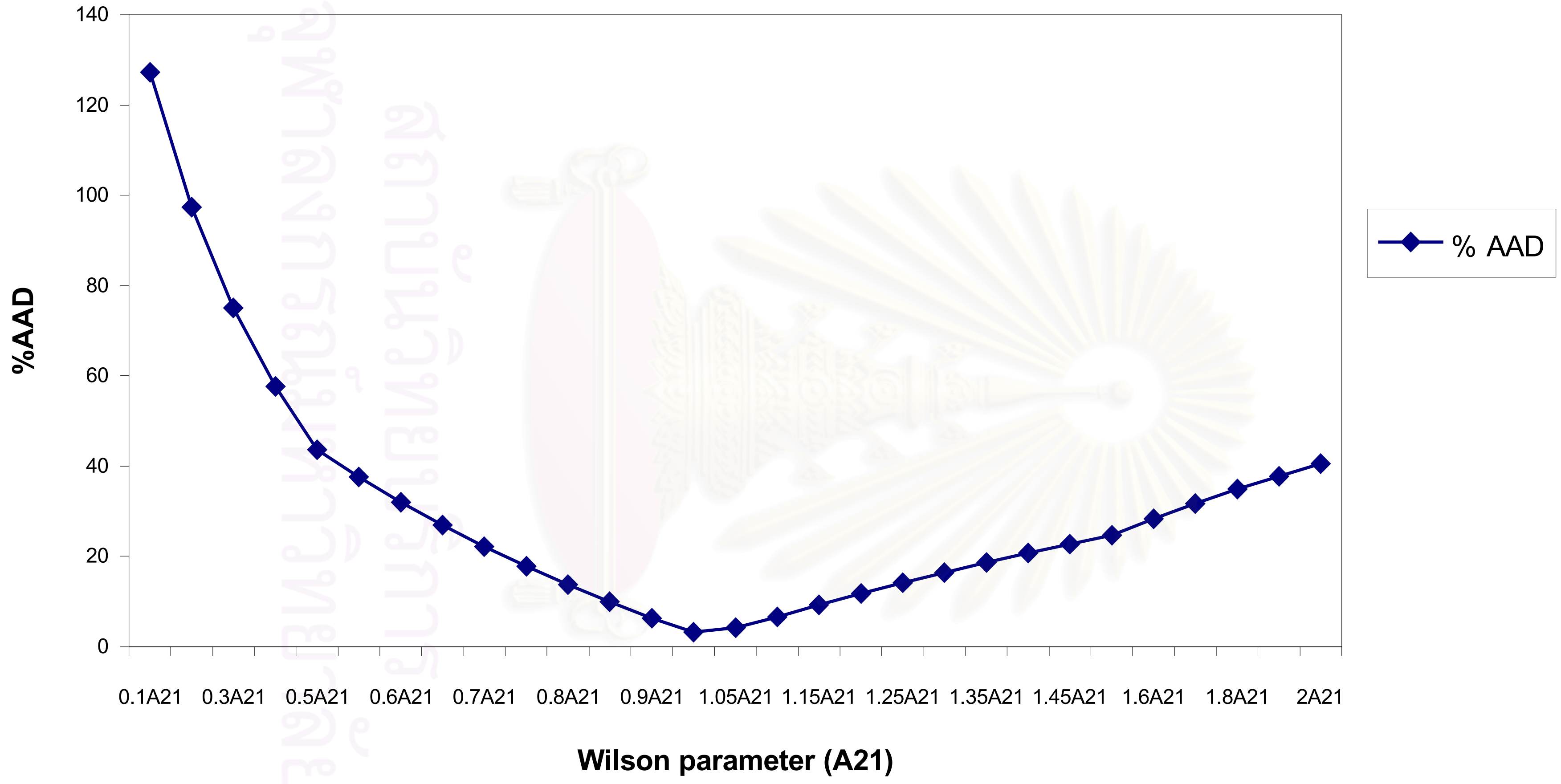


Figure5.9 %Average Absolute Deviation (%AAD) of the K-value by varying Wilson parameter (A21).

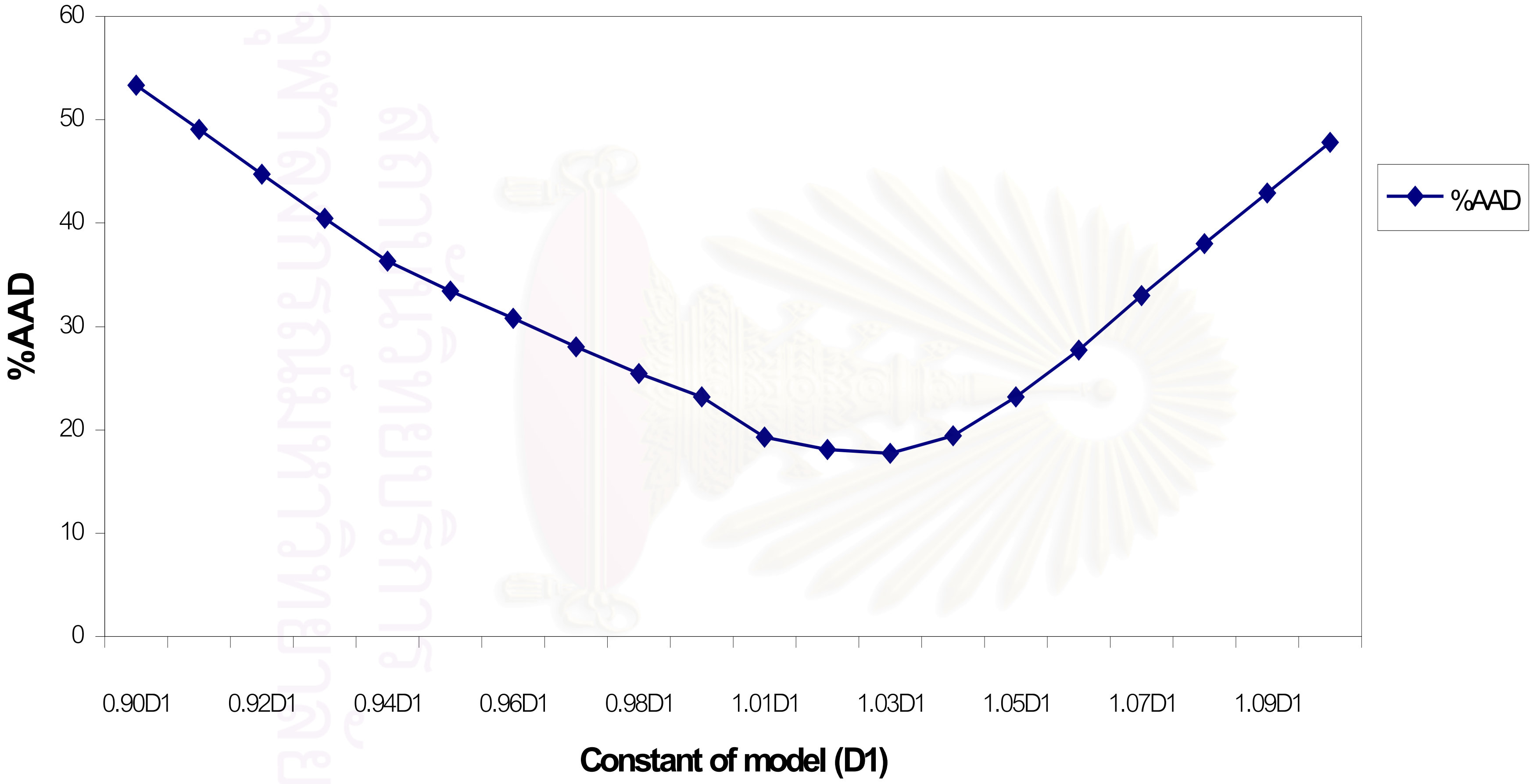


Figure5.10 %Average Absolute Deviation (%AAD) of enthalpy model at any constant(D1) of model.

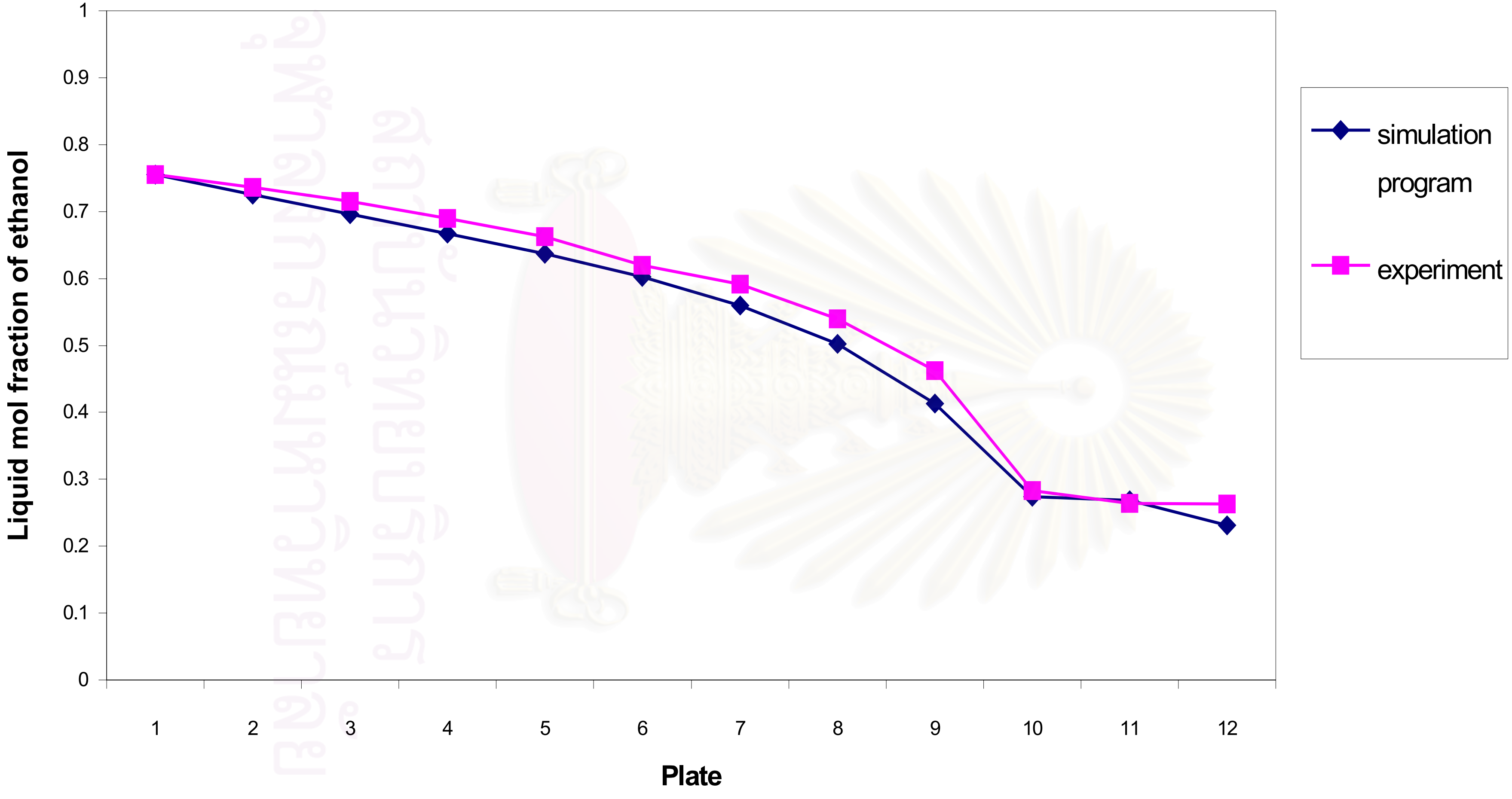


Figure5.11 The liquid composition (x1) profile of distillation data of ethanol(1)+water(2) from simulation program and experiment.

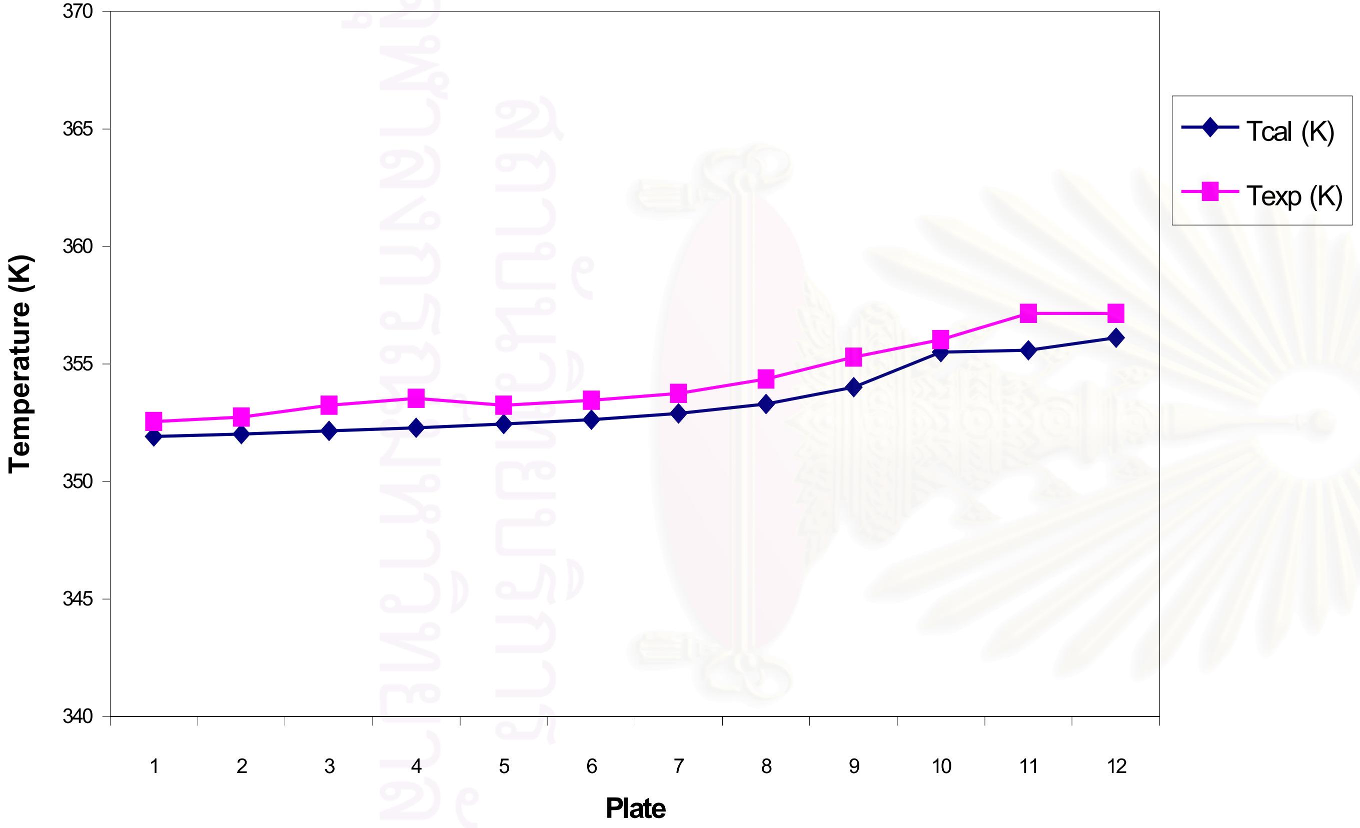


Figure5.12 The temperature profile of distillation simulation data of ethanol(1)+water(2) from simulation program and experiment.

5.3.1 Effect of Inaccuracy in Vapor-Liquid Equilibrium Constant (K-value) on Distillation Simulation

The vapor-liquid equilibrium constant (K-value) depends on the activity coefficient model, vapor pressure model and fugacity coefficient model. These models are normally accurate except only the activity coefficient model. If an inaccurate activity coefficient model is used, the vapor-liquid equilibrium constant (K-value) is also inaccurate.

To study the effect of inaccuracy in vapor-liquid equilibrium constant (K-value), the A_{21} parameter value of the activity coefficient model is varied. Table5.36 shows the %AAD at any error parameter of the model. The %AAD of the K-value (or activity coefficient model)at approximate ±6%, ±9%, ±22%, ±32% and ±37% are used in distillation simulation.

The results of distillation simulation at any %AAD are shown in Table5.60-Table5.69 in AppendixG. The effect of the inaccuracy K-value on the composition profile of distillation simulation can be presented in Figure5.13 and Figure5.14. And the effect of the inaccuracy K-value on the temperature profile of distillation simulation can be presented in Figure5.15 and Figure5.16.

It can be concluded that error in the K-value will have great effect on distillation simulation result. Distillation simulation with error in K-value exceeding ±9% should not be acceptable.

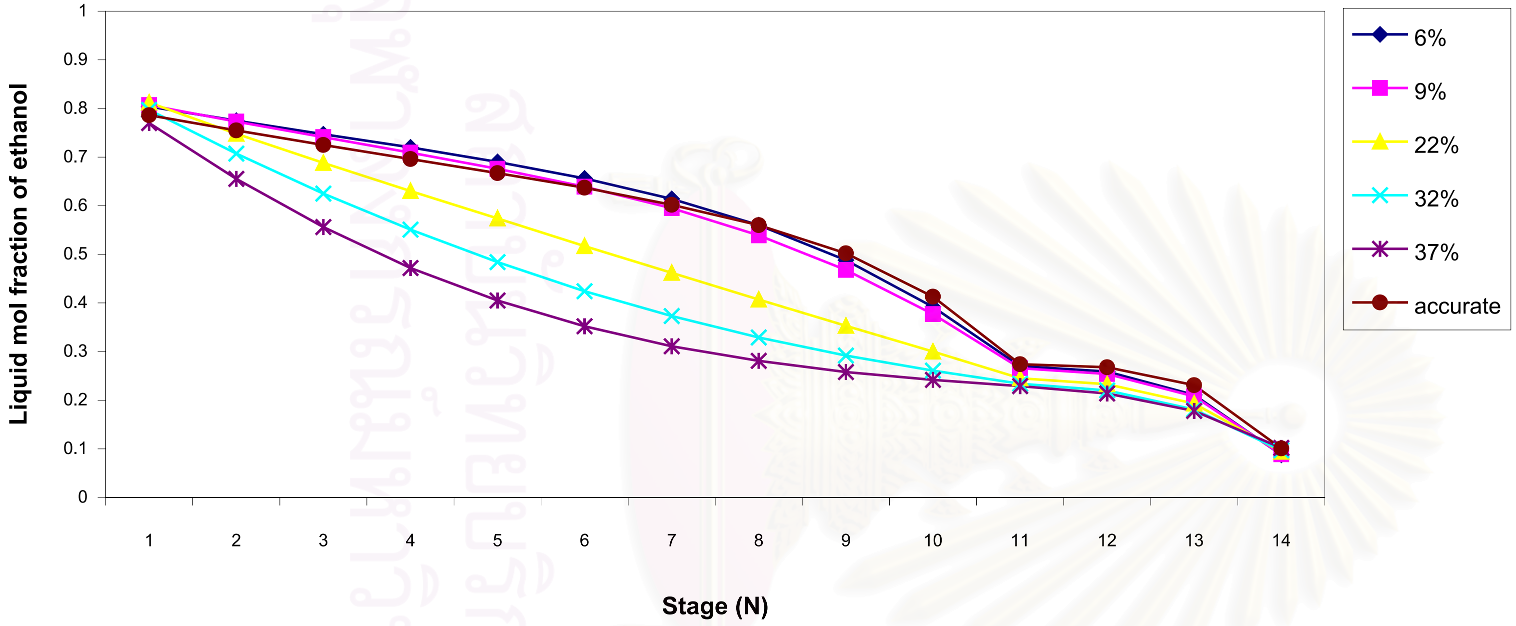


Figure5.13 The liquid composition (x1) profile by varying %AAD of the K-value in increasing Wilson parameter (A21).

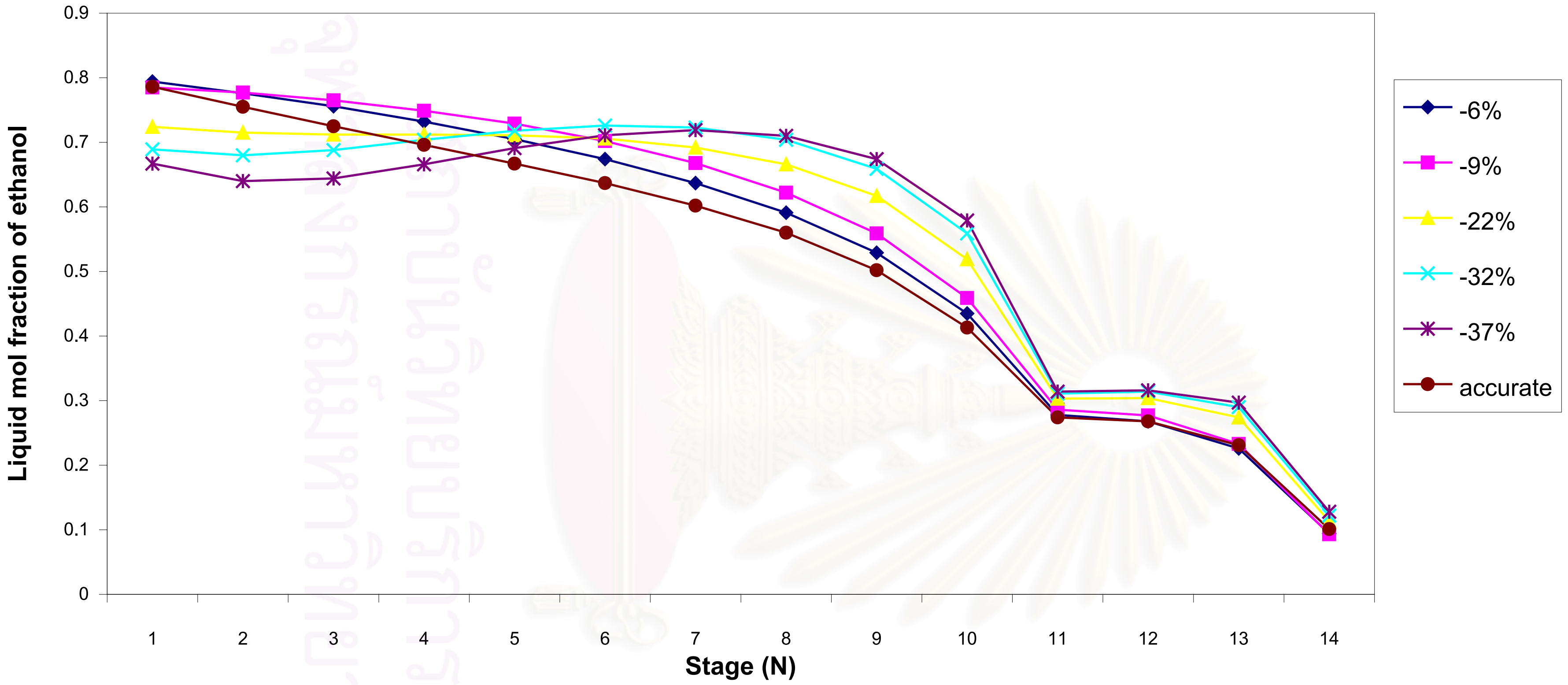


Figure5.14 The liquid composition (x1) profile by varying %AAD of the K-value in decreasing Wilson parameter (A21).

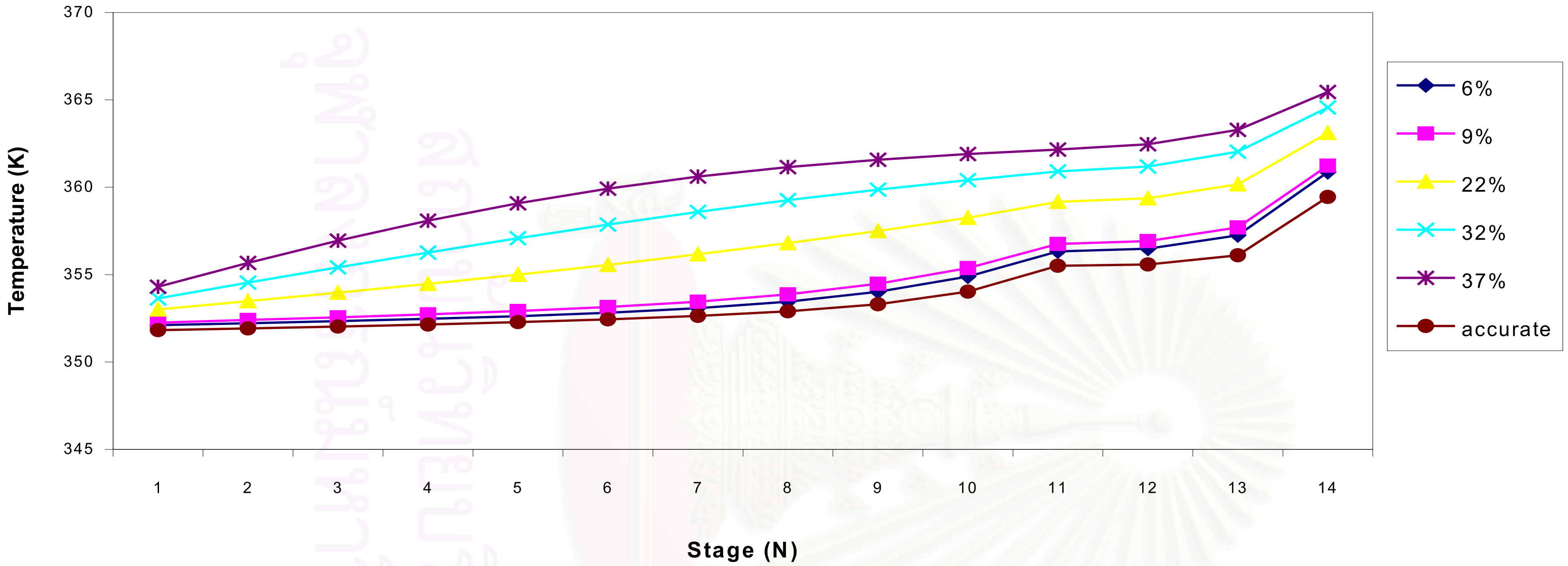


Figure5.15 The temperature profile by varying %AAD of the K-value in increasing Wilson parameter (A21).

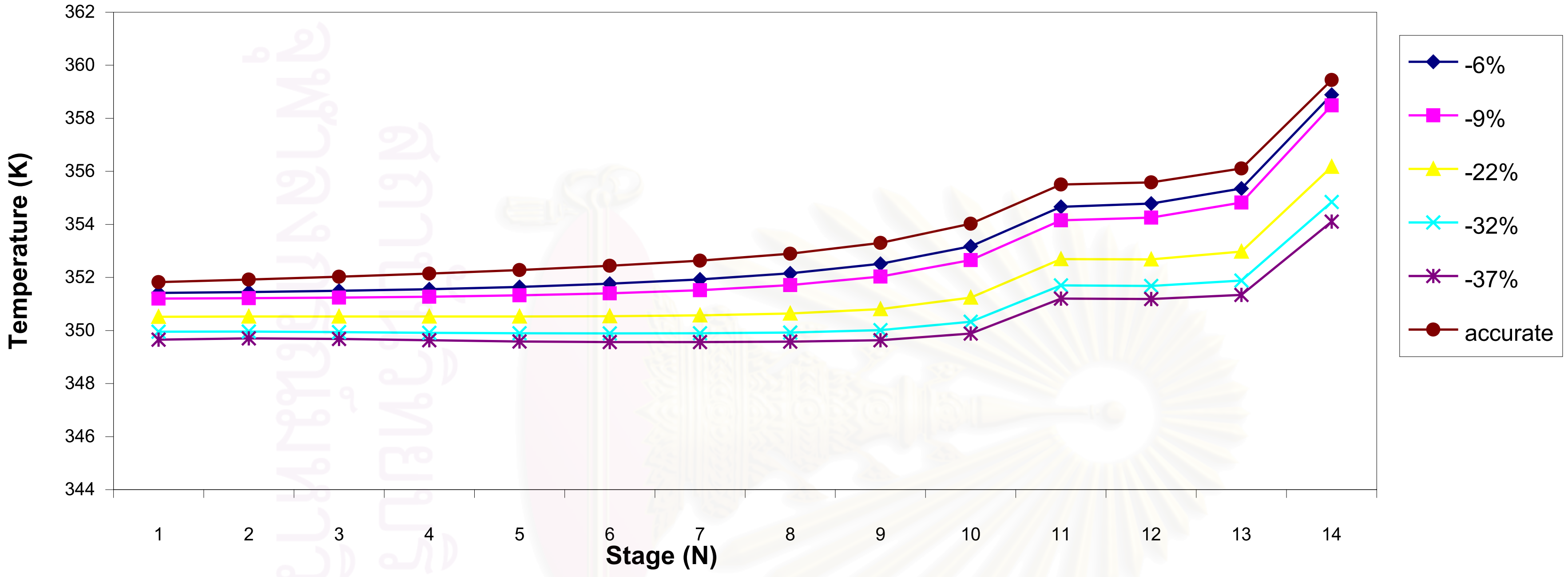


Figure5.16 The temperature profile by varying %AAD of the K-value in decreasing Wilson parameter (A21).

5.3.2 Effect of Inaccuracy in Enthalpy Model on Distillation Simulation

The accuracy of enthalpy model depends on the constants of model. There are many constants in the enthalpy model. To study the effect of inaccuracy in the enthalpy model, the constant (D_1) in the model is selected to vary at any error. Table5.57 shows the %AAD at any error constant (D_1) of model. To observe the effect of inaccuracy in the enthalpy model. The %AAD of enthalpy model at approximate ±23%, ±28%, ±33% and ±37% are chosen for simulation in this works.

The results of simulation distillation with various %AAD in enthalpy model are shown in Table5.74-Table5.81 in AppendixG. The effect of inaccuracy of the enthalpy model on the composition profile can be presented in Figure5.17 and Figure5.18. The effect of inaccuracy of the enthalpy model on the temperature profile is presented in Figure5.19 and Figure5.20.

It can be stated that the distillation simulation is not sensitive to the error in enthalpy. Even though the error is as high as ±37%, the simulation result is still acceptable.

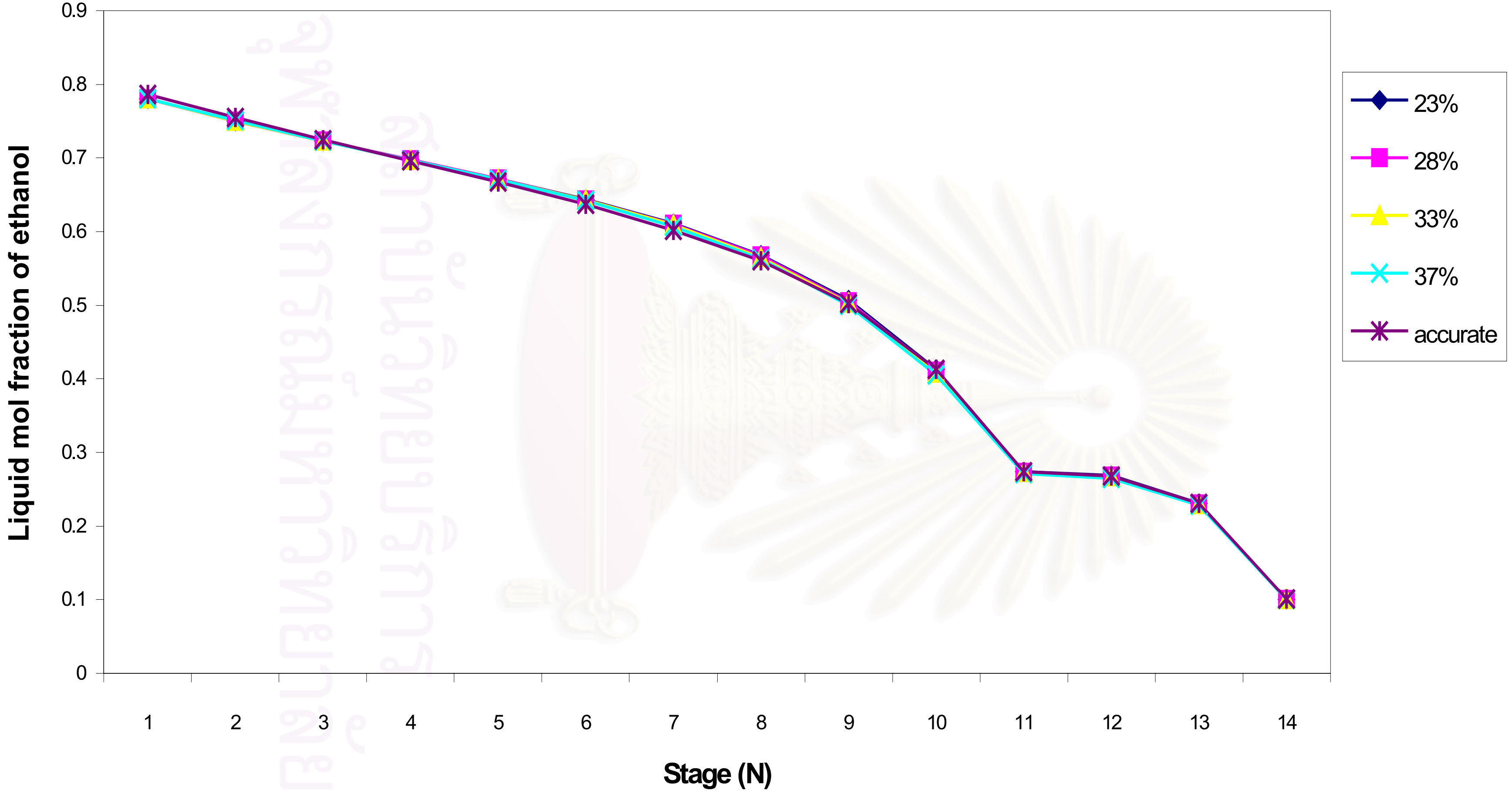


Figure5.17 The liquid composition (x1) by varying %AAD of the enthalpy model in increasing constant (D1).

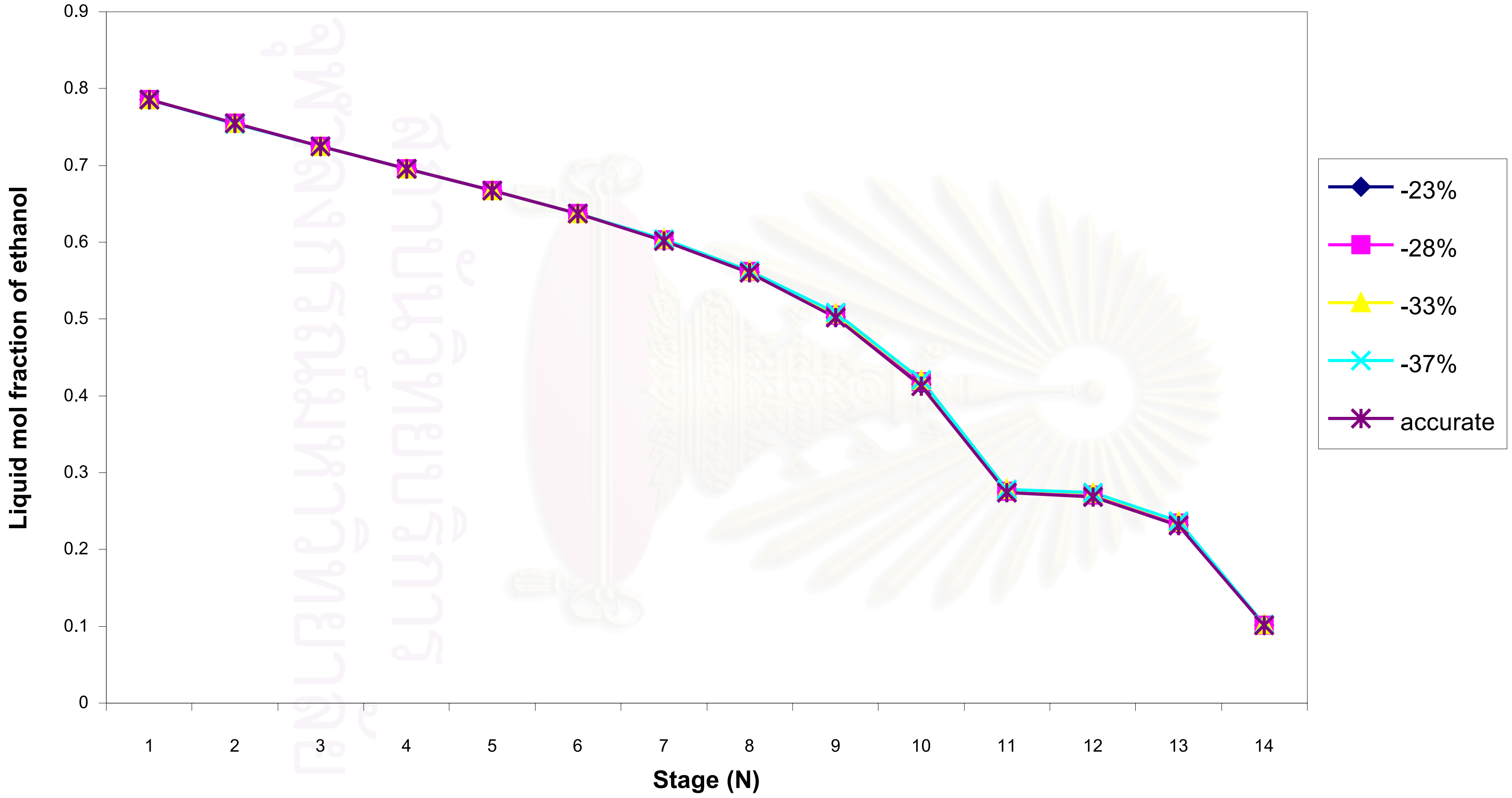


Figure5.18 The liquid composition (x1) profile by varying %AAD of the enthalpy model in decreasing constant (D1).

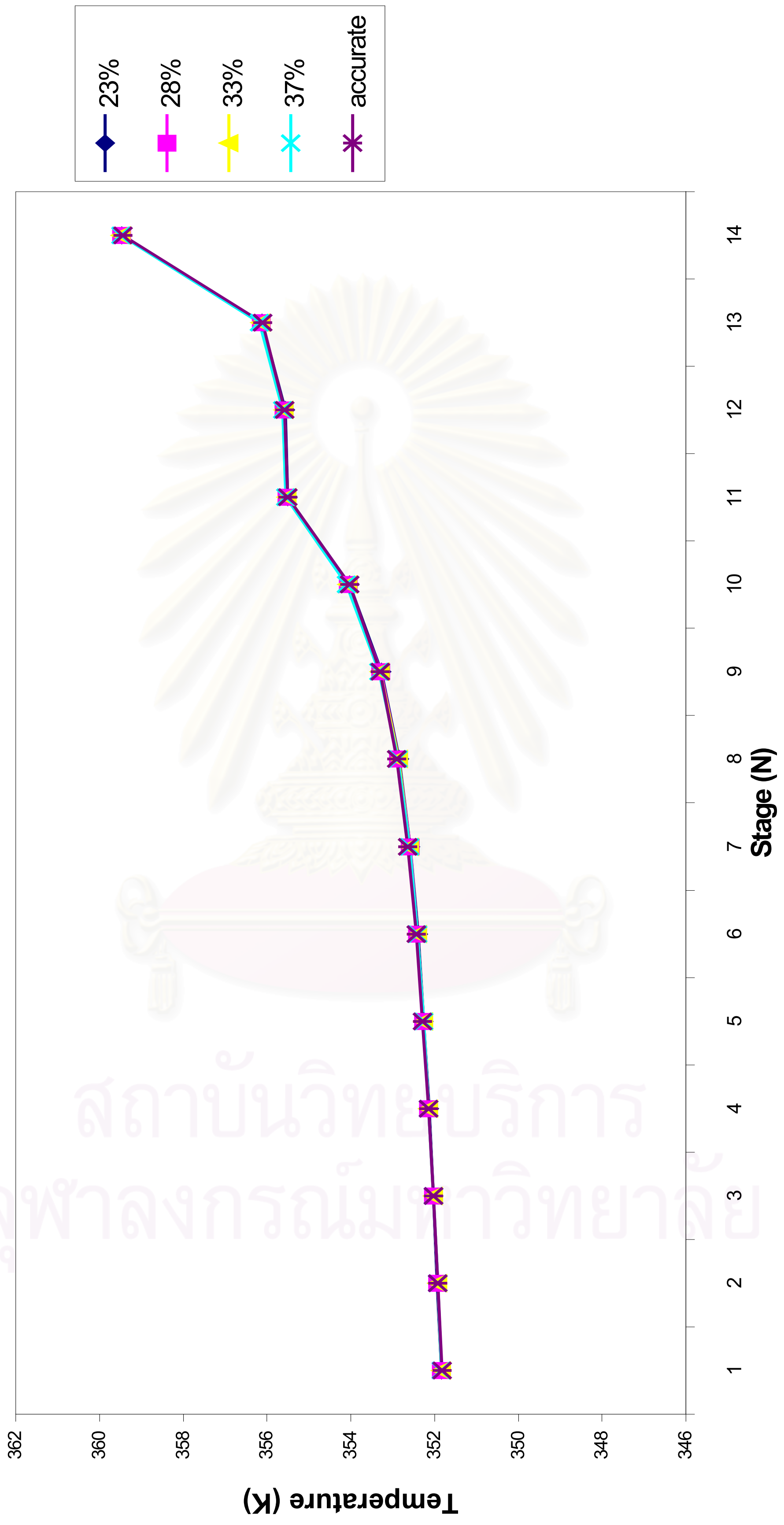


Figure5.19 The temperature profile by varying %AAD of the enthalpy model in increasing constant (D1).

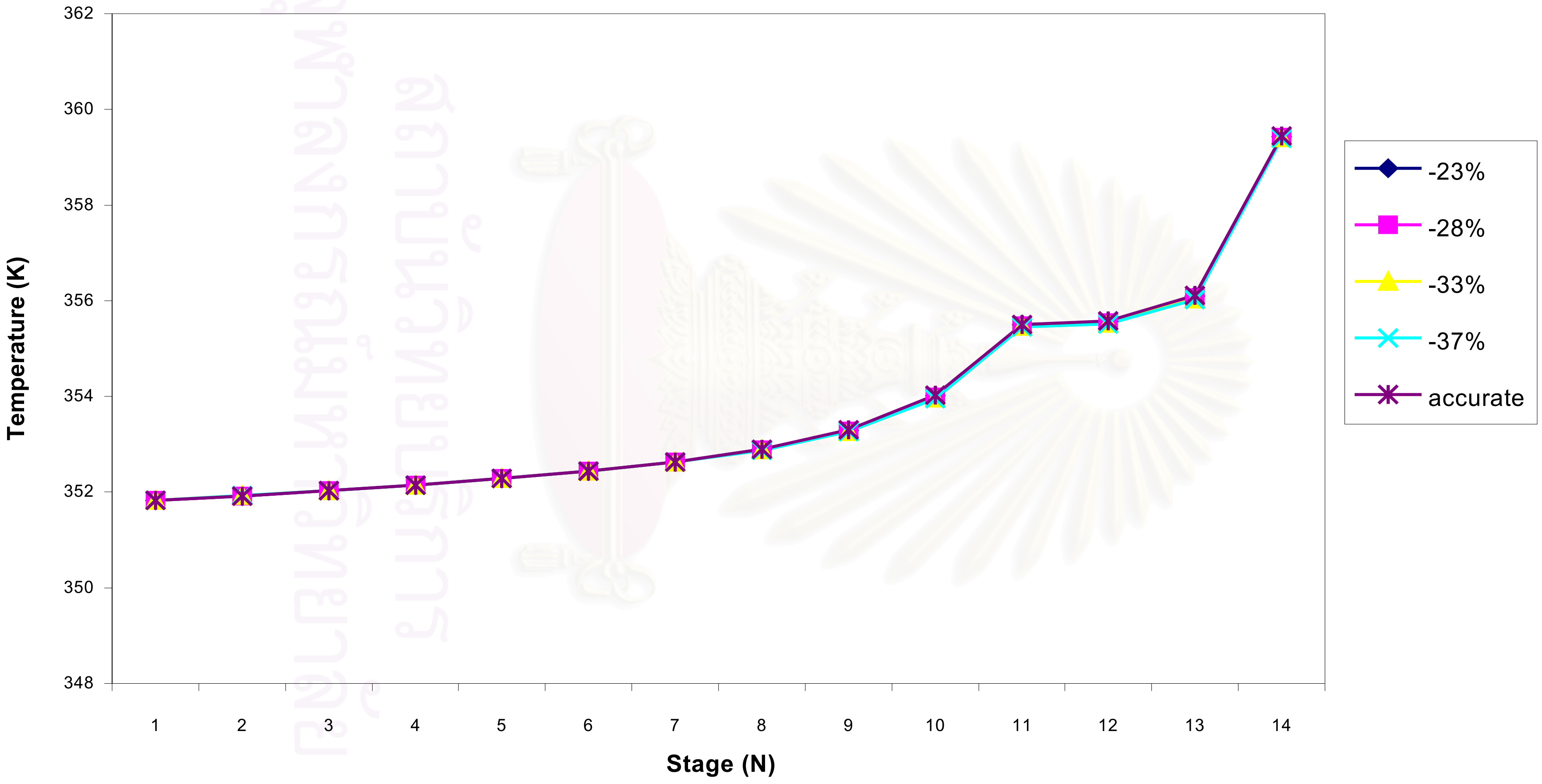


Figure5.20 The temperature profile by varying %AAD of the enthalpy model in decreasing constant (D1).

5.3.3 Effect of Reflux Ratio on Distillation Simulation

From the previous section, distillation simulation is not sensitive to error in enthalpy. Therefore, only inaccuracy in K-value is considered in this section. This section is to study the effect of reflux ratio on the distillation simulation with error in K-value. The additional reflux ratios used are those obtained by varying ±10% value of experimental reflux ratio of 1.7. Their values are 1.9 and 1.55.The results of simulation distillation are shown in Table5.86-Table5.95 in AppendixG. In Table5.96-Table5.99 and Figure5.21-Figure5.24, the %AAD of effect of reflux ratio on the composition profile at %AAD of K-value ±9% and ±22% are shown. The temperature profile of distillation simulation are presented in Table5.100-Table5.103 and Figure5.25-Figure5.28 respectively.

It can be concluded that at a specified error of K-value, error in the result of distillation simulation slightly increases as the reflux ratio decreases. However, if the percent error in K-value is less than 10, there is almost no effect of reflux ratio on the simulation result.

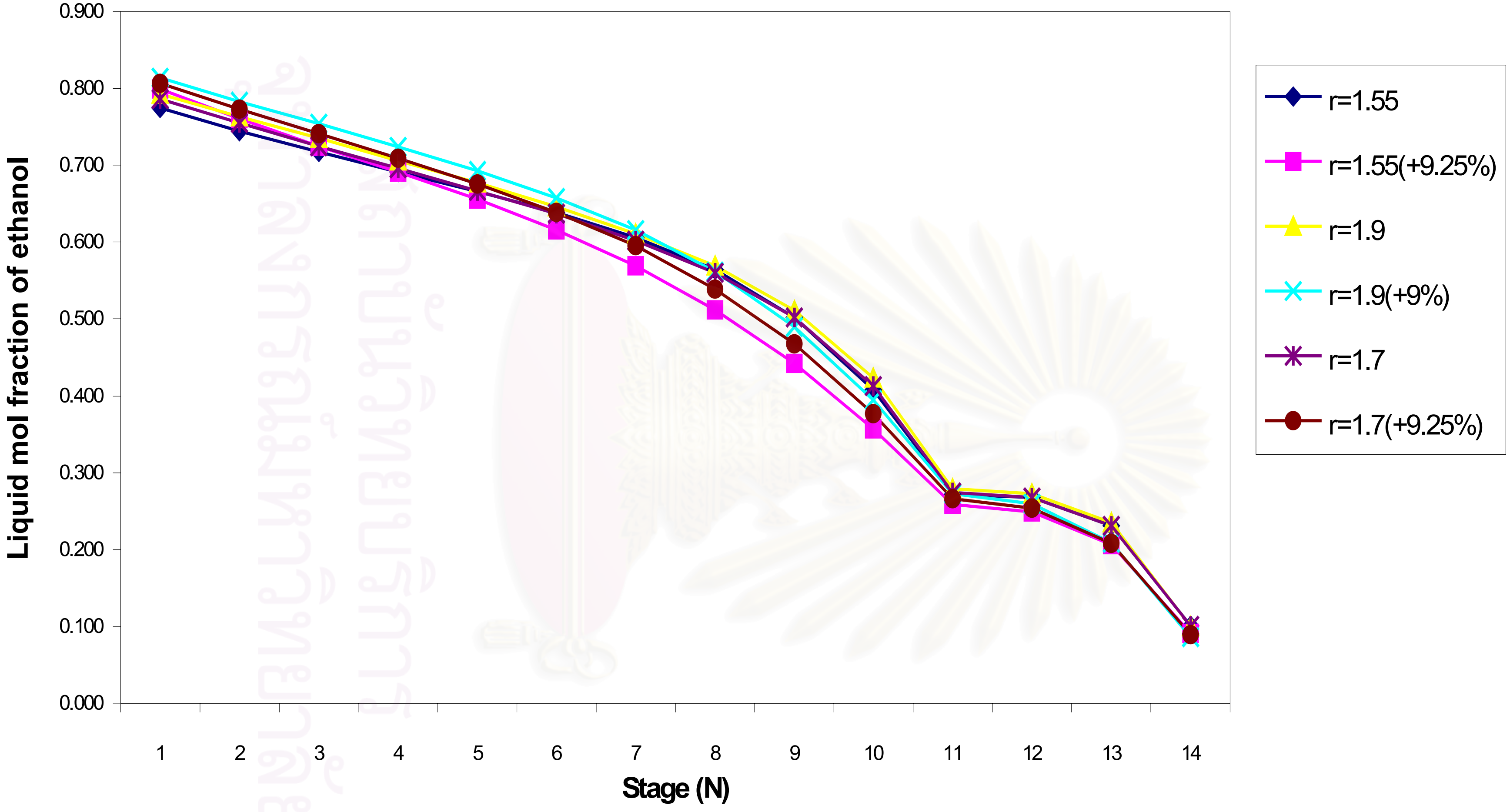


Figure5.21 The composition profile by varying the reflux ratio at %AAD of K-value +9.25%.

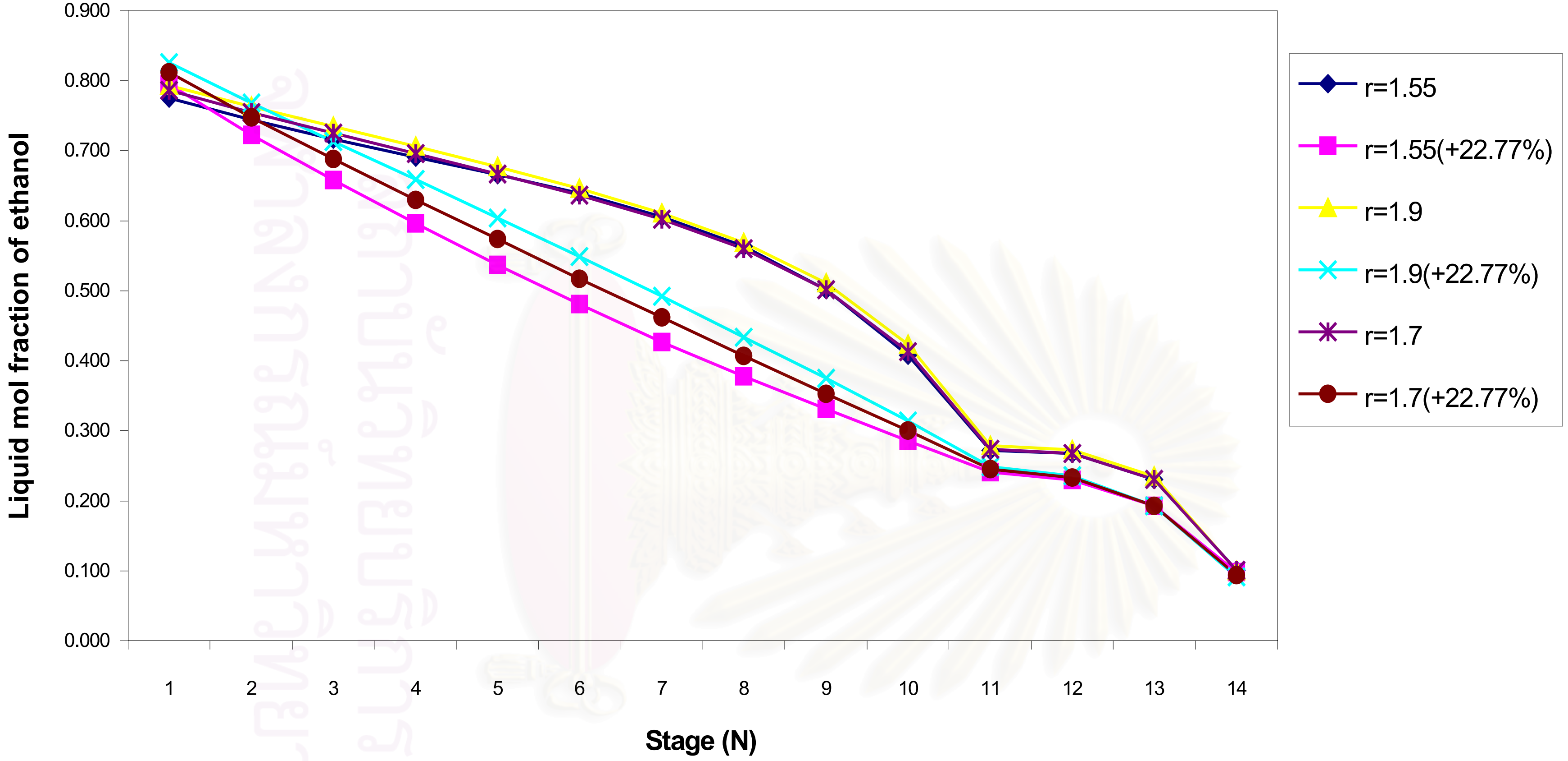


Figure5.22 The composition profile by varying reflux ratio at %AAD of K-value +22.77%.

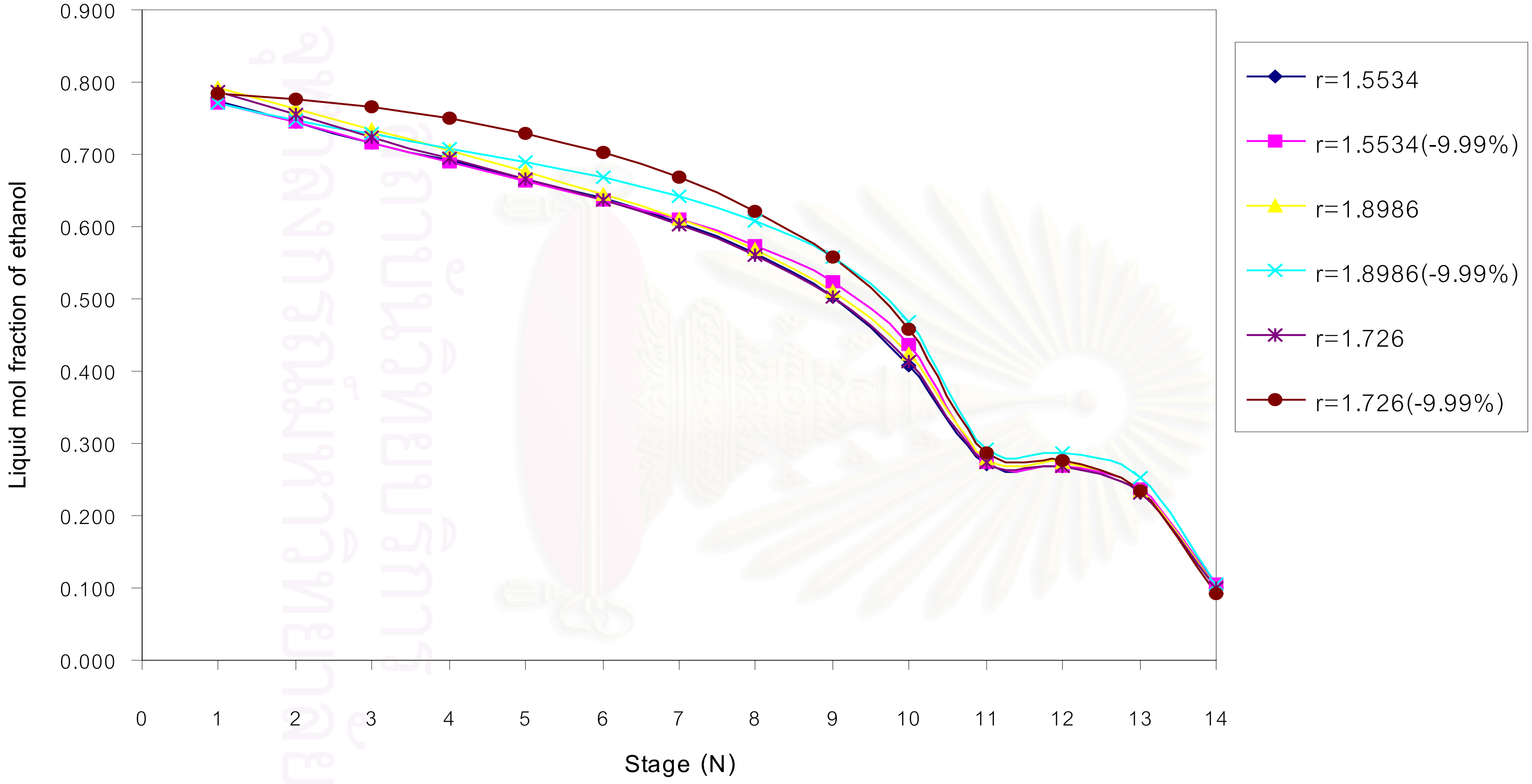


Figure5.23 The composition (x1) profile by varying reflux ratio at %AAD of K-value –9.99%.

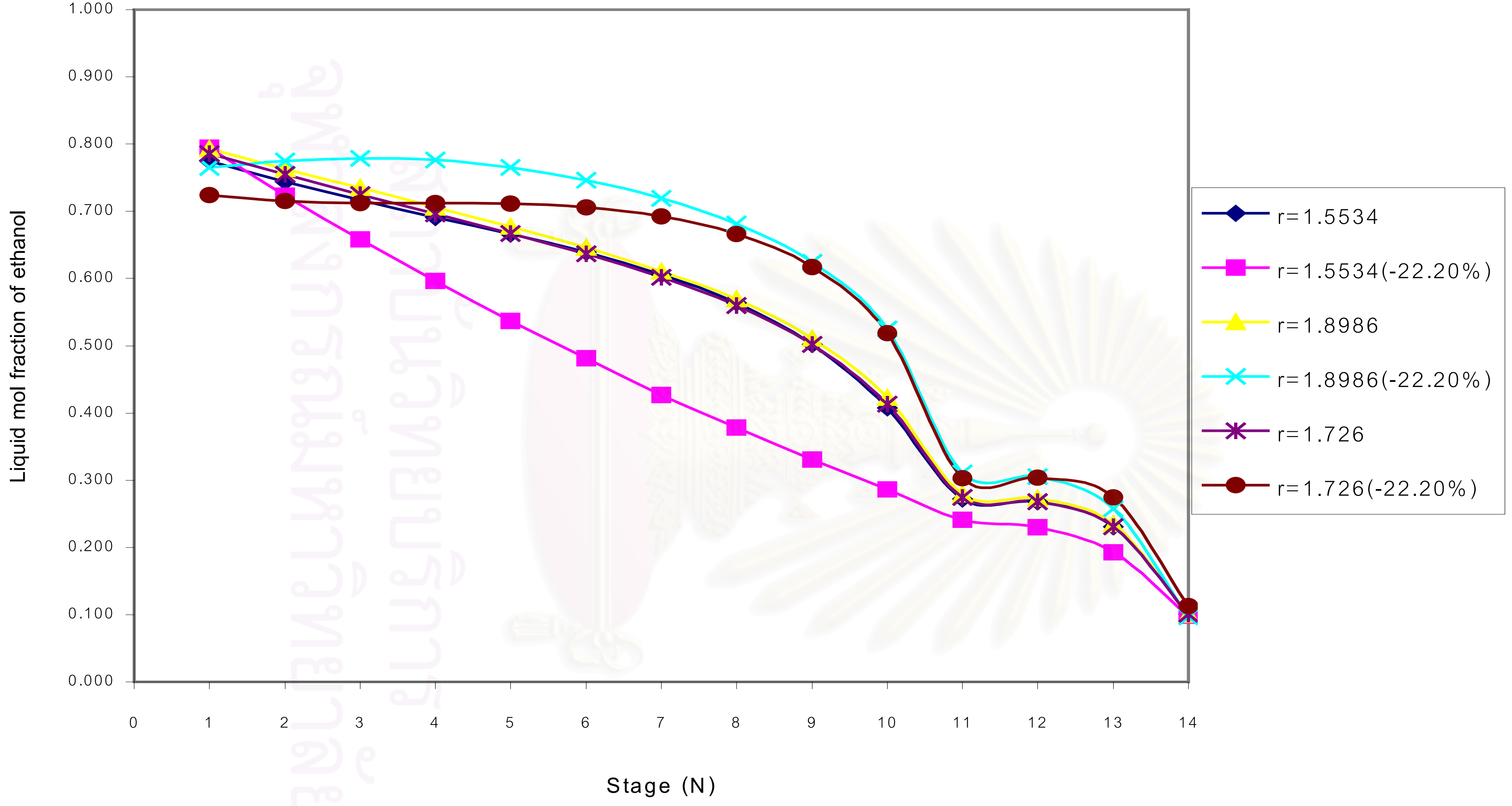


Figure5.24 The composition (x1) profile by varying reflux ratio at %AAD of K-value –22.20%.

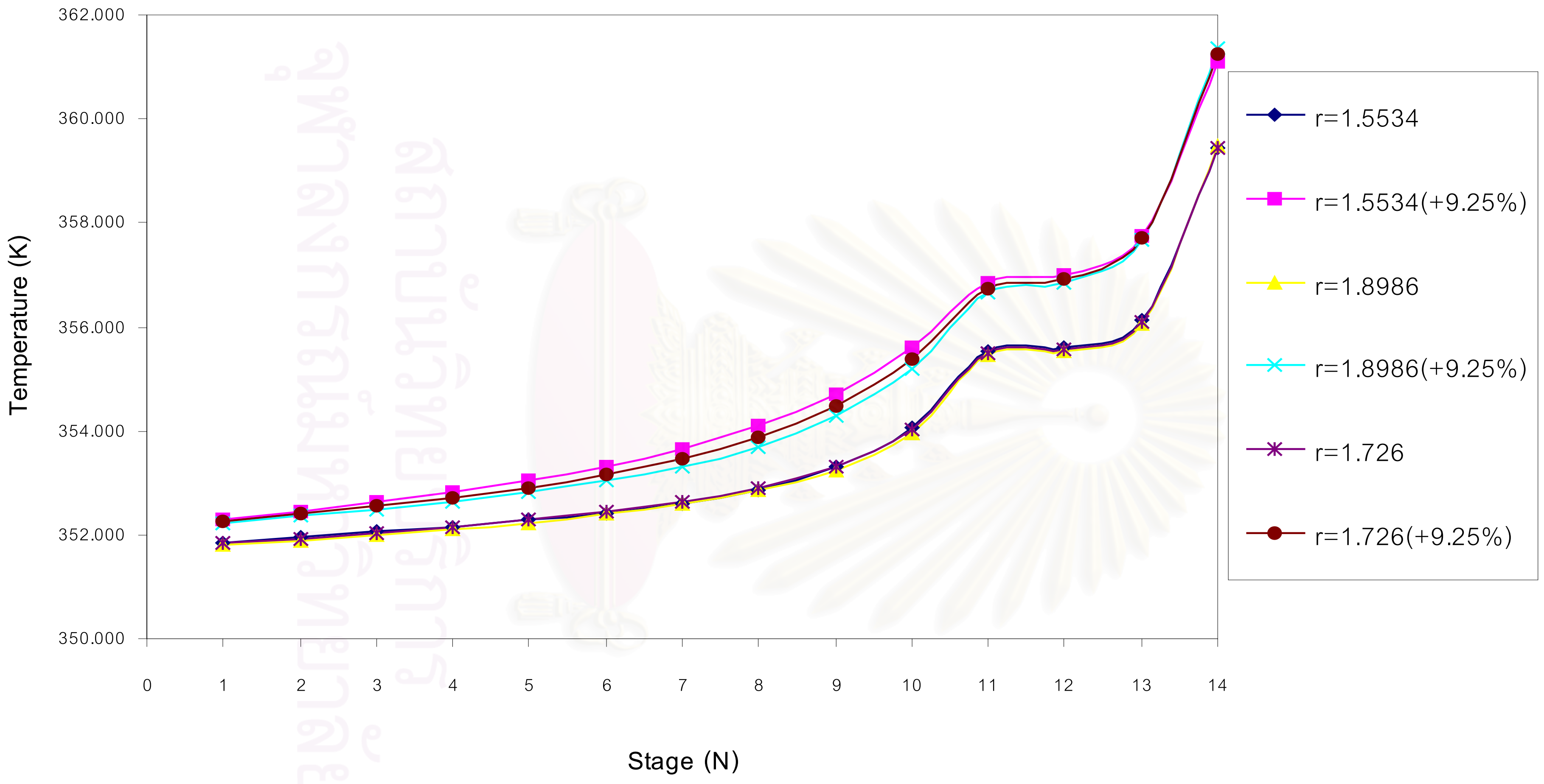


Figure5.25 The temperature profile by varying reflux ratio at %AAD of K-value +9.25%.

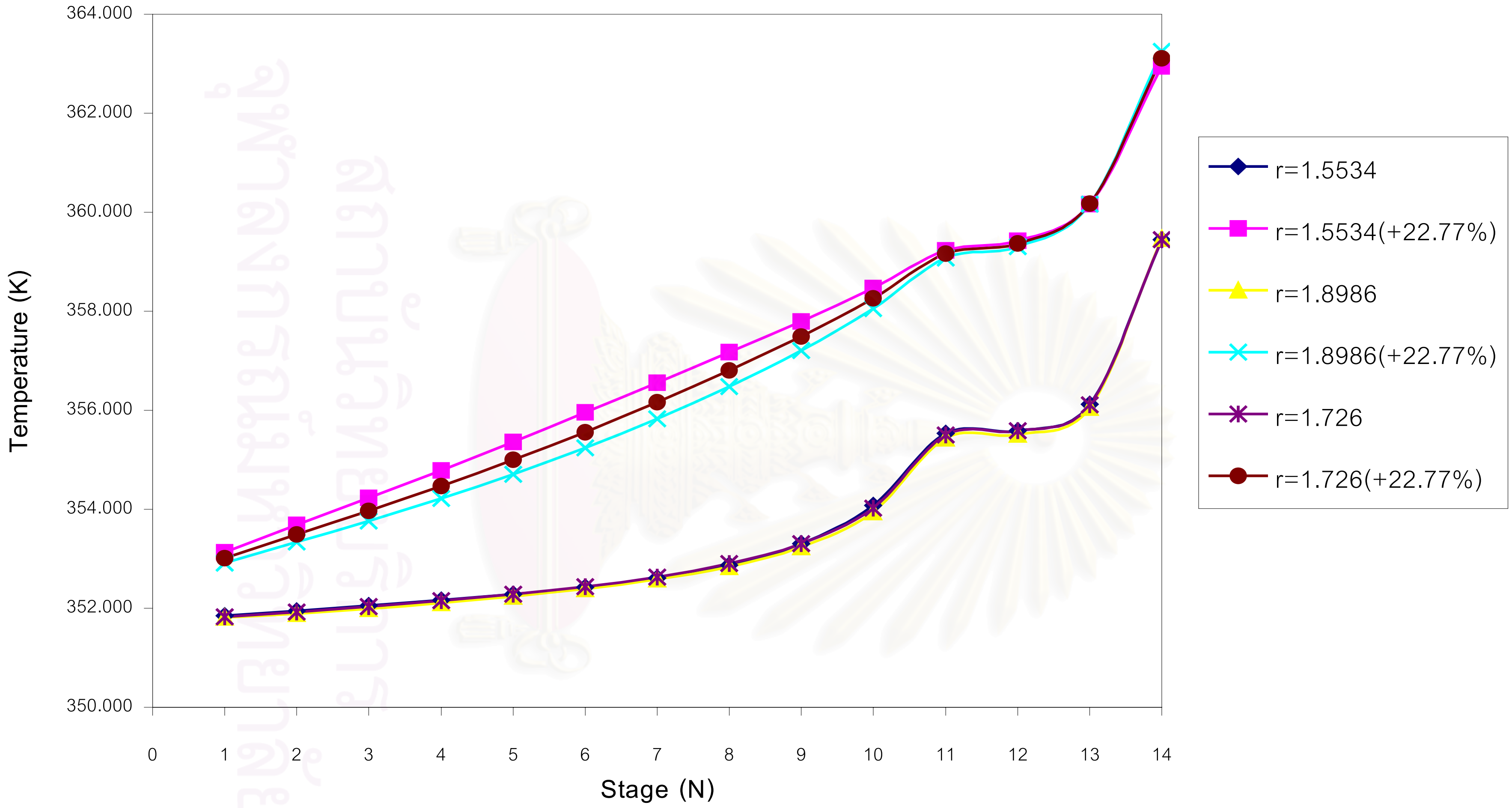


Figure5.26 The temperature profile by varying reflux ratio at %AAD of K-value +22.77%.

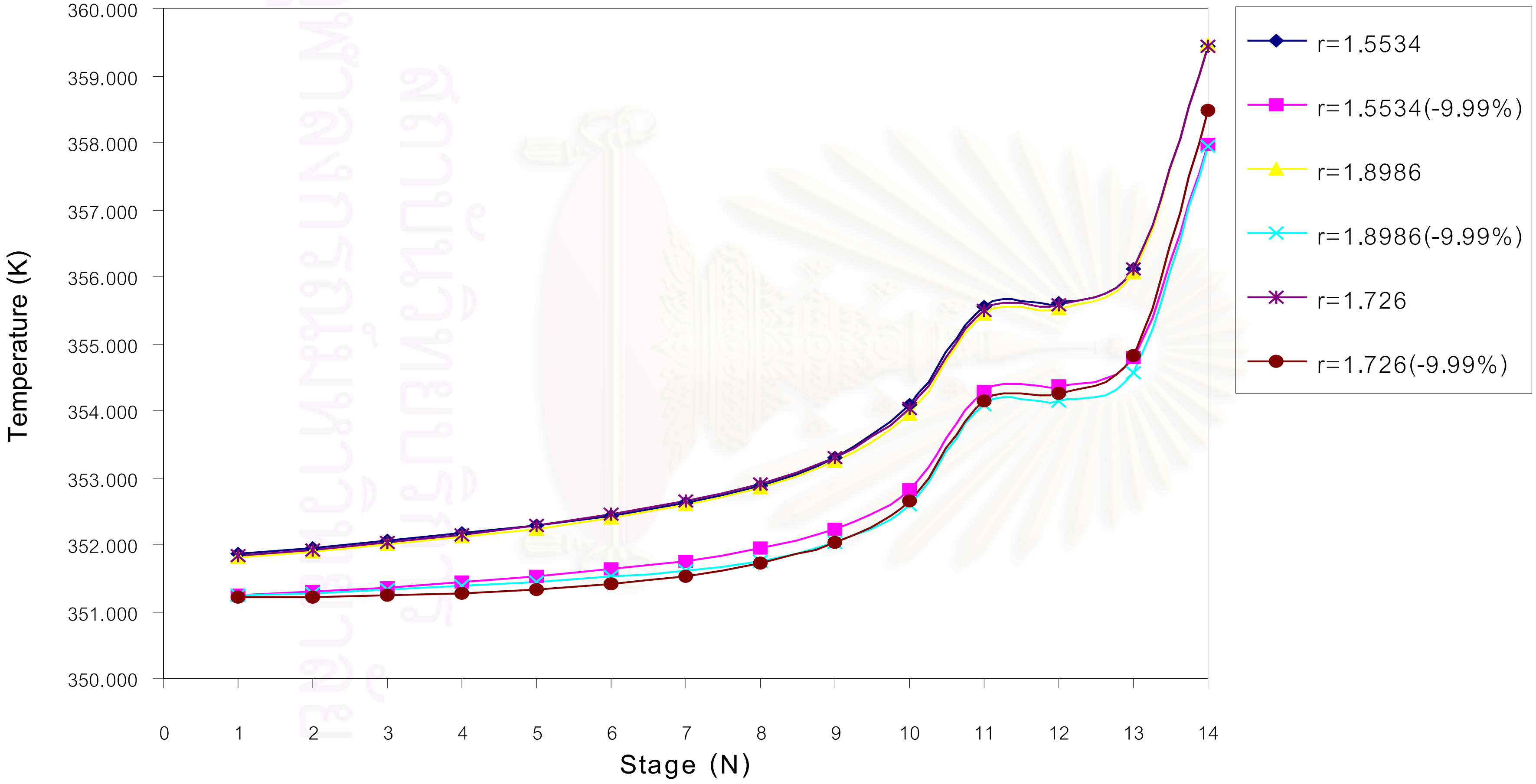


Figure5.27 The temperature profile by varying reflux ratio at %AAD of K-value –9.99%.

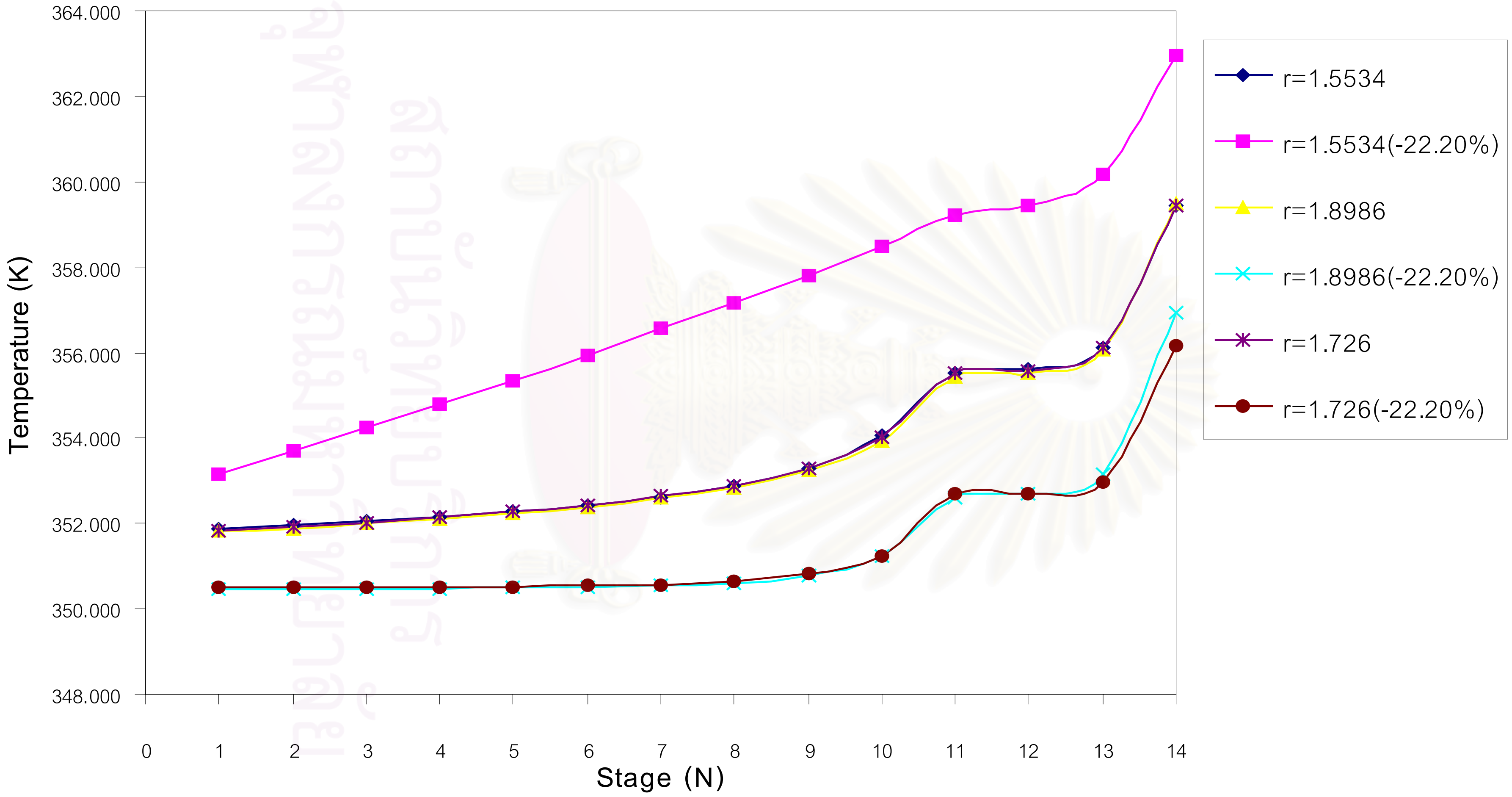


Figure5.28 The temperature profile by varying reflux ratio at %AAD of K-value –22.20%.

5.3.4 Effect of Number of Stage on Distillation Simulation

Only inaccuracy in K-value is considered in this section. This section is to study the effect of the number of stage on the distillation simulation. The number of stage are 10, 14 and 20. At that number of stages, the feed stage are 8, 11 and 15 respectively. The results of simulation distillation by varying the number of stage at any feed stage are shown in Table5.104-Table5.113 in AppendixG. The effect of the number of stage on the composition profile and the temperature profile of distillation simulation is presented in Figure5.29-Figure5.32.

It can be concluded that at a specified error in K-value, the error in simulated temperature profile is independent of numbers of equilibrium stages. But this is not true in the case of composition profile. With positive error in K-value, the error in simulated composition profile decreases with decreasing number of stages ; but with negative error in K-value, the error in simulated composition profile increases with decreasing number of stages.

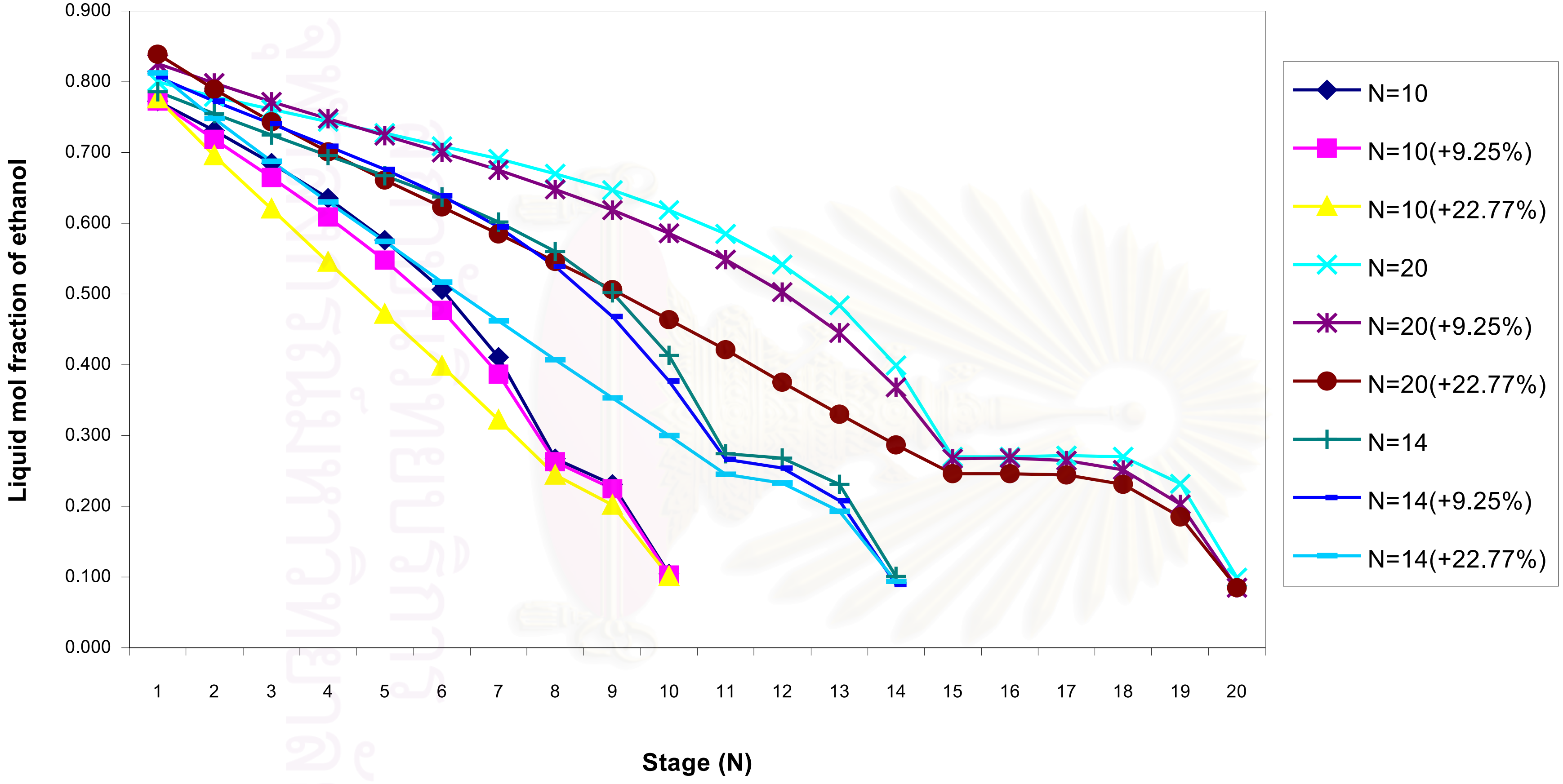


Figure5.29 The composition profile by varying number of stage at %AAD of K-value +9.25%, +22.77%.

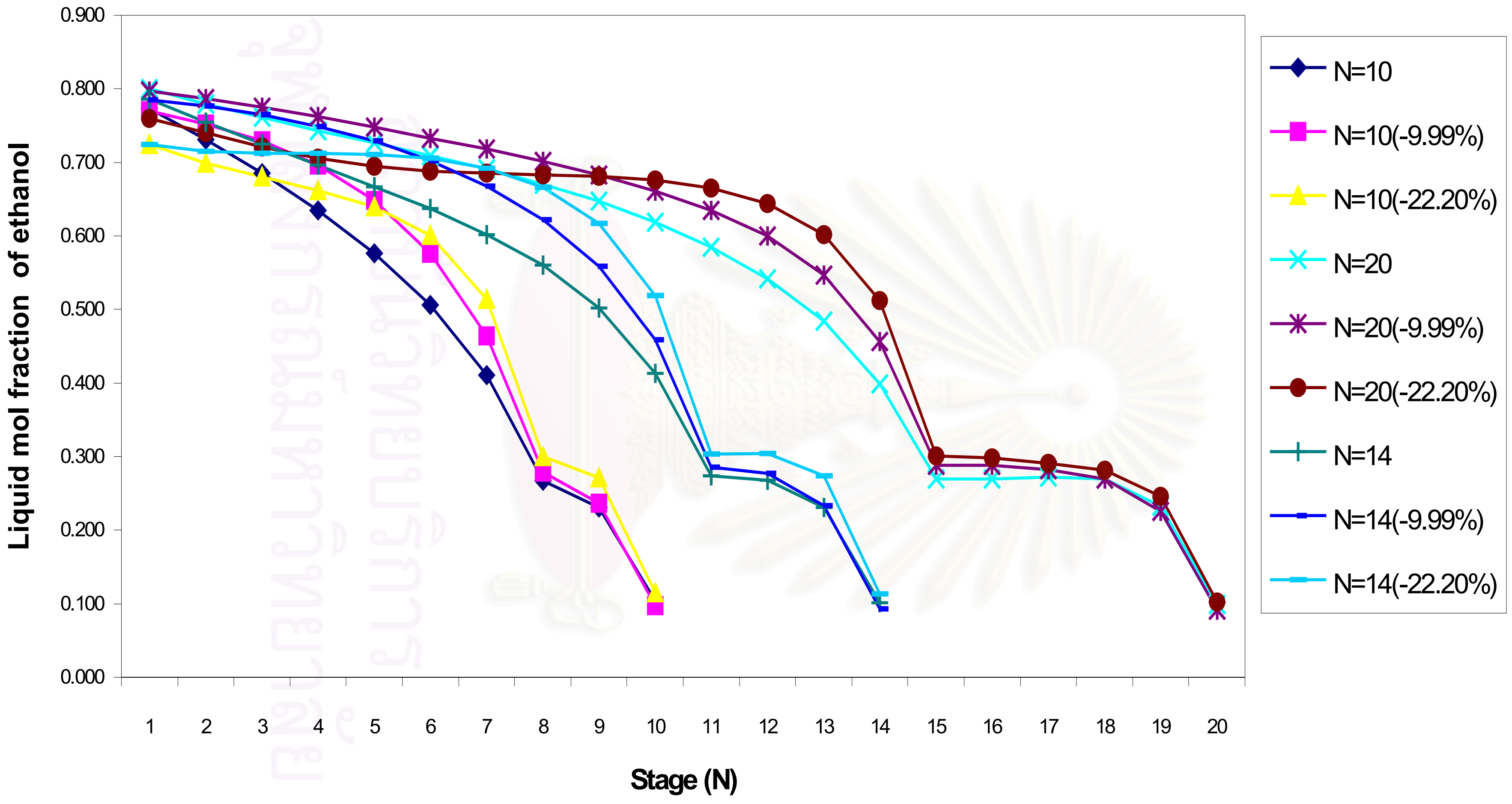


Figure5.30 The composition profile by varying number of stage at %AAD of K-value -9.99%, -22.20%.

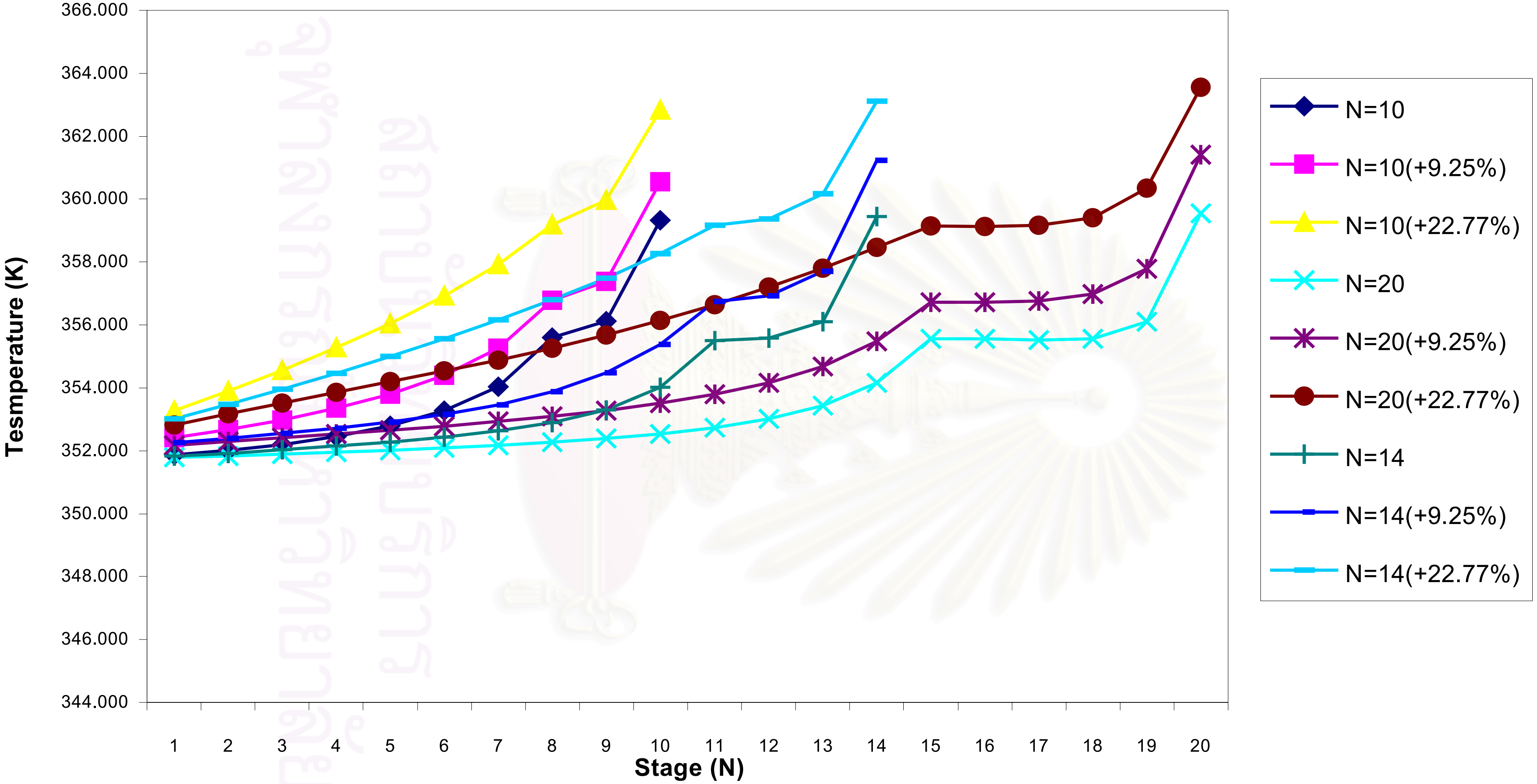


Figure5.31 The temperature profile by varying the number of stage at %AAD of K-value +9.25%, +22.77%.

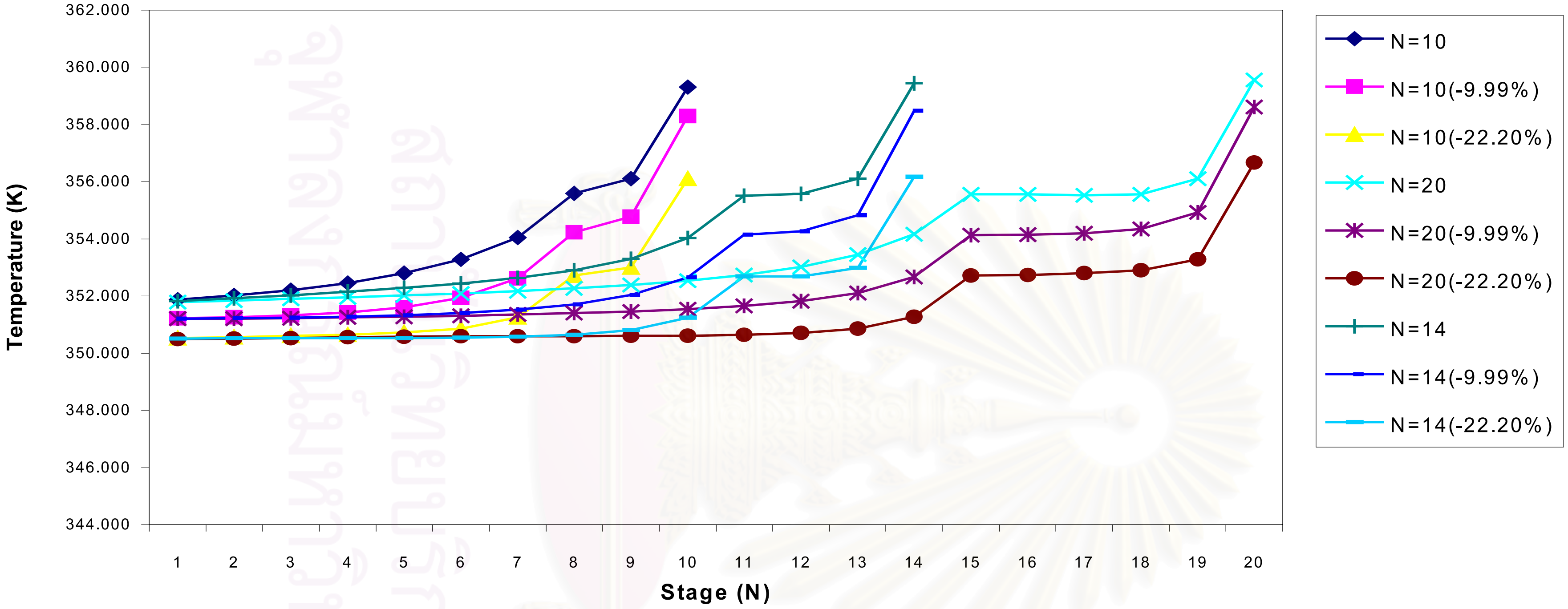


Figure5.32 The temperature profile by varying the number of stage at %AAD of K-value –9.99%, -22.20%.

CHAPTER 6

CONCLUSION

1. Accurate distillation simulation result can be obtained when accurate thermodynamic property models are used.
2. For ethanol+water system, the error in the K-value will have great effect on distillation simulation result: Distillation simulation with error in K-value exceeding ± 9% should not be acceptable.
3. For ethanol+water system, the distillation simulation is not sensitive to the error in enthalpy. Even though the error is as high as ±37%, the simulation result is still acceptable.
4. At a specified error of K-value, error in the result of distillation simulation slightly increases as the reflux ratio decreases. However, if the percent error in K-value is less than 10, there is almost no effect of reflux ratio on the simulation result.
5. At a specified error in K-value, the error in simulated temperature profile is independent of numbers of equilibrium stages. But this is not true in the case of composition profile. With positive error in K-value, the error in simulated composition profile decreases with decreasing number of stages ; but with negative error in K-value, the error in simulated composition profile increases with decreasing number of stages.

   Therefore, for good simulation results, the accurate K-value must be used.

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APPENDICES

Appendix A

Computer program for distillation simulation

Distillation simulation program:

```
import java.lang.*;
import java.text.*;
import java.io.*;
public class Test {  //   ethanol(1)+water(2)
  int m = 0; // row - stage of distillation
  int n = 0; // column - number of x
  int maxit = 10000;
  int maxouter = 50;
  double TOL = 0.01;
  double tsq = (double) (1.0/3.0);
  double T0 = 273.15;
  /** from input **/
  double[] E = null;
  double[][] x = null;
  double[][] y = null;
  double[] Z = null;
  double[] T = null;
  double[] TC = null;
  double[] PC = null;
  double[] V = null;
  double[] VC = null;
  double[] nu = null;
  double[] omegah = null;
  double[] mu = null;
  double[] a = null;
  double[] b = null;
  double[] c = null;
  double[] d = null;
  double[] d1 = null;
```

```
double[] d2 = null;
double[] d3 = null;
double[] d4 = null;
double[] c2 = null;
double[] c3 = null;
double[] c4 = null;
double[] c5 = null;
double[] omega = null;
double F = 0;
double D = 0;
double B = 0;
double Hf = 0;
double P = 0;
int f = 0;
double r = 0;
double _initT0 = 0;
 /** from calculate **/
double[][] K = null;
double[] L = null;
double[][] gamma = null;
double[][] psat = null;
double[][] phi = null;
double[][] Bv = null;
double[] A12 = null;
double[] A21 = null;
double[] lamda12 = null;
double[] lamda21 = null;
double[] a12 = null;
double[] a21 = null;
double[] Hl = null;
double[] Hv = null;
PrintWriter _out = null;
String infile = null;
String outfile = null;
```

```
public Test(String infile, String outfile) { // reading parameter and constants
  m = 14; n = 2;
  // init cal
  E = new double[m];
  K = new double[m][n];
  L =new double[m];
  gamma = new double[m][n];
  psat = new double[m][n];
  phi = new double[m][n];
  Bv = new double[n][n];
  V = new double[m];
  A12 = new double[m];
  A21 = new double[m];
  lamda12 = new double[m];
  lamda21 = new double[m];
  a12 = new double[m];
  a21 = new double[m];
  Hl = new double[m];
  Hv = new double[m];
  E = new double [m];
  E[0]=1.0;     E[1]=1.0;      E[2]=0.54;
  E[3]=0.61;    E[4]=0.66;     E[5]=0.86;
  E[6]=0.55;    E[7]=0.77;     E[8]=0.88;
  E[9]=0.74;    E[10]=0.7;     E[11]=0.57;
  E[12]=0.48;   E[13]=1.0;

  x = new double[m][n];
  for(int i=0;i<m;i++) {
    for(int j=0;j<n;j++) {
      x[i][j] = 0.5;
    }
  }
  y = new double[m][n];
  for(int i=0;i<m;i++) {
```

```
    for(int j=0;j<n;j++) {
      y[i][j] = 0.5;
    }
  }

  T = new double[m];
  for(int i=0;i<m;i++) {
    T[i] = 300;
  }
  Z = new double[n];
  Z[1]  = 0.771;  Z[0] = 0.229;
  TC  = new double[n];
  TC[1] = 647.3; TC[0] = 513.9;
  PC = new double[n];
  PC[1] = 221.2; PC[0] = 61.4;
  V = new double[m];
 for(int i=0;i<m;i++) {
   V[i] = 100;
  }
 VC = new double[n];
 VC[1] = 57.1; VC[0] = 167.1;
 nu = new double[n];
 nu[1] = 0; nu[0] = 1.10;
 omegah = new double[n];
 omegah[1] = 0.01; omegah[0] = 0.152;
 mu = new double[n];
 mu[1] = 1.83; mu[0] = 1.69;
  a = new double[n];
  a[1] = -7.76451; a[0] = -8.51838;
  b = new double[n];
  b[1] = 1.45838; b[0] = 0.34163;
  c = new double[n];
  c[1] = -2.7758; c[0] = -5.73683;
  d = new double[n];
```

```
  d[1] = -1.23303; d[0] = 8.32581;
  d1 = new double[n];
  d1[1] = 25.573; d1[0] = -744.60;
  d2 = new double[n];
  d2[1] = 897.86; d2[0] = 21117;
  d3 = new double[n];
  d3[1] = 0.013705; d3[0] = -0.046915;
  d4 = new double[n];
  d4[1] = 0.15825; d4[0] = 132.08;
  c2 = new double[n];
  c2[1] = -7004.8; c2[0] = -3465.9;
  c3 = new double[n];
  c3[1] = 0.0035888; c3[0] = -0.062301;
  c4 = new double[n];
  c4[1] = -6.6689; c4[0] = 20.468;
  c5 = new double[n];
  c5[1] = -0.00000085054; c5[0] = 0.000020664;
  omega = new double[n];
  omega[1] = 0.344; omega[0] = 0.644;
  F = 196.3;  //mol/min
  D = 37.51; // mol/min
  B = 158.8; // mol/min
  Hf= 7.252316;// kJ/mol
  P = 1.013;
  f = 10;
  r = 1.726;
  _initT0 = 350.0; // Kelvin
        this.infile = infile;
        this.outfile = outfile;
  try {
    _out = new PrintWriter(new FileOutputStream(outfile), true);
  } catch(Exception e) {System.exit(0);}
};
```

```
public void process() {  // main procedure
  boolean feasible = false;
  for(int loop=0;loop<maxouter;loop++) {
    for(int i=0;i<m;i++) {
      calK(T[i] ,i);
    }
    System.out.println("Finish Cal K");
    calX();
    System.out.println("Finish Cal X");
    double[] oldT = new double[m];
    System.arraycopy(T, 0, oldT, 0, T.length);
    System.out.println("Finish arr cpy");
    for(int i=0;i<m;i++) {
      T[i] = calT(_initT0, i);
    }
    System.out.println("Finish Cal T");
    double ssr = 0;
    for(int i=0;i<m;i++) {
     ssr += Math.pow(Math.abs(T[i]-oldT[i]), 2);
    }
    if(ssr <= 0.01*m) {
      output();
      feasible = true;
      break;
    }
    else {
      caly();
      calV();
    }
  }
  System.out.println("Finish All");
  if(!feasible)
  System.out.println("Infeasible solution");
};
```

```
  private void calV() {   // calculate vapor phase flow rate(V)
    double R= 8.31451;//j/molK
    V[0] = 0.0;
    L[0] = r*D;
    V[1] = D+L[0];
    for(int i=0;i<m;i++) {
//cal Hl
      double suml1=0;
      double suml2=0;
   for(int j=0;j<n;j++) {
   suml1 = suml1 + x[i][j] *
         ( (d1[j]*(T[i] - T0)) + (d2[j]*Math.log(T[i]/T0)) +
           (d3[j]*(Math.pow(T[i], 2)- Math.pow(T0, 2))/2) +
           (d4[j]*(T[i]*Math.log(T[i]) - (T0*Math.log(T0)) + T0 - T[i]))
         );
   suml2 = suml2 + x[i][j] *
         ( (-c2[j]) + (c3[j]*Math.pow(T[i], 2)) +
           (c4[j]*T[i]) + (2*c5[j]*Math.pow(T[i], 3))
         );
    } //end j
   lamda21[i] = (4.8515167*T[i])+2092.03;
   lamda12[i] = (18.736775*T[i]) -4822.41;
   a21[i] =( 0.001933167*T[i] + 0.2035);
   a12[i] = -0.00087525*T[i] +0.477;
   double he = x[i][0] * x[i][1] *
            ( ((lamda12[i]*a12[i])/(x[i][0]+(a12[i]*x[i][1]))) +
             ((lamda21[i]*a21[i])/((a21[i]*x[i][0]) + x[i][1]))
            );
 // cal Hlo
      double sumlo1=0;
      double sumlo2=0;
```

```
   for(int j=0;j<n;j++) {
   sumlo1 = sumlo1 + x[i][j] *
           ( (d1[j]*(273.15 - T0)) + (d2[j]*Math.log(273.15/T0)) +
             (d3[j]*(Math.pow(273.15, 2)- Math.pow(T0, 2))/2) +
             (d4[j]*(273.15*Math.log(273.15) - (T0*Math.log(T0)) + T0 - 273.15))
           );
   sumlo2 = sumlo2 + x[i][j] *
           ( (-c2[j]) + (c3[j]*Math.pow(273.15, 2)) +
             (c4[j]*273.15) + (2*c5[j]*Math.pow(273.15, 3))
           );
   } //end j
   double  lamdao21 = (4.8515167*273.15)+2092.03;
   double  lamdao12 = (18.736775*273.15) -4822.41;
   double  ao21 = (0.001933167*273.15 + 0.2035);
   double  ao12 = -0.00087525*273.15 +0.477;
   double heo = x[i][0] * x[i][1] *
               ( ((lamdao12*ao12)/(x[i][0]+(ao12*x[i][1]))) +
                 ((lamdao21*ao21)/((ao21*x[i][0]) + x[i][1]))
               );
   double Hlo = ( sumlo1 - R*sumlo2 +heo )/1000 ;

   Hl[i] = ( (suml1 - R*suml2 +he )/1000 )-Hlo ; // kJ/mol

// cal Hv
      double sumv1 = 0;
      double sumv2 = 0;
      double[] TR = new double[n];
   for(int j=0;j<n;j++) {
        TR[j]=T[i]/TC[j];
   sumv1 = sumv1 + y[i][j] *
          ( (d1[j]*(T[i] - T0)) + (d2[j]*Math.log(T[i]/T0)) +
            (d3[j]*(Math.pow(T[i], 2)- Math.pow(T0, 2))/2) +
            (d4[j]*(T[i]*Math.log(T[i]) - (T0*Math.log(T0)) + T0 - T[i]))
          );
```

```
    sumv2 = sumv2 + (TC[j]*(P/PC[j]))*(-(0.1445+(0.073*omega[j]))+
            ((0.660-(0.92*omega[j]))/TR[j])+((0.4155+(1.50*omega[j]))/
            Math.pow(TR[j],2))+((0.0484+(0.388*omega[j]))/Math.pow(TR[j],3))
            + ((0.0657*omega[j])/Math.pow(TR[j],8))
            );
      } //end j
   double latent =(  (x[i][0]*(R*4300))+(x[i][1]*(R*4400)) )/1000;

    Hv[i] = (( sumv1 -R*sumv2 )/1000)+ latent + Hl[i] ;  //kJ/mol
  } // end for i
 // cal V
     for(int i=2;i<m;i++) {
        double[]av=new double[m];
       double[]bv=new double[m];
       double[]cv=new double[m];
       av[i-1] = Hl[i-2] - Hv[i-1];
       bv[i-1] = Hv[i] - Hl[i-1];
       double tmpF = i-1==f?F:0;
       double tmpf = i-2>=f?F:0;
       double tmpHf = i-1==f?Hf:0;
       cv[i-1] = ((tmpf-D)*(Hl[i-1] - Hl[i-2])) + (tmpF*(Hl[i-1]-tmpHf));

       V[i] = (cv[i-1] - (av[i-1]*V[i-1]))/bv[i-1];
     }
   };
```

```
  private double calT(double initT0, int i) { //calculate Temperature
    double h = 0.1;
    double initT1 = initT0 + 0.1;
    double fx0 = 0;
    calK(initT0, i);
    for(int j=0;j<n;j++) {
      fx0 += K[i][j] * x[i][j];
    }
      fx0 = fx0-1;

    double fx1 = 0;
    calK(initT1, i);
    for(int j=0;j<n;j++) {
      fx1 += K[i][j] * x[i][j];
    }
    fx1 = fx1-1;
    //start iterative
    for(int j=1;j<maxit;j++) {
      double zz = initT0 -(fx0 / ((fx1-fx0)/h));
output();
double retP = zz;
System.out.println("Finish step1");
      if(Math.abs(zz-initT0) < TOL) {
System.out.println("found sol");
        return retP;
      }
      else {
System.out.println("not found sol, begin iteration: "+Math.abs(zz-initT0));
        return calT(retP, i);
      }
    }
    return 0;
  };
```

```
 private void calK(double mT, int i) {  // calculate K-value
    A21[i] =( (0.001933167*mT)+0.2035);
    A12[i] =( (-0.00087525*mT)+0.477 )  ;
    gamma[i][0] = (Math.exp(x[i][1]*((A12[i]/(x[i][0]+(A12[i]*x[i][1])))-
                        (A21[i]/((A21[i]*x[i][0])+x[i][1])))
                      ) ) /   (x[i][0]+(A12[i]*x[i][1]));
    gamma[i][1] = (Math.exp(-x[i][0]*((A12[i]/(x[i][0]+(A12[i]*x[i][1])))-
                        (A21[i]/((A21[i]*x[i][0])+x[i][1])))
                      ) ) /   (x[i][1]+(A21[i]*x[i][0]));
// complete cal gamma (activitycoefficient)

// begin to cal psat
    for(int j=0;j<n;j++) {
      double tao = 1 - (mT / TC[j]);
      double logpsat = (1/(1-tao)) *
                    ( (a[j]*tao) + (b[j]*tao*Math.sqrt(tao)) +
                      (c[j]*Math.pow(tao, 3)) + (d[j]*Math.pow(tao, 6)) );
      psat[i][j] = Math.exp(logpsat) * PC[j];
    } // end for j
// Cal B(second virial coefficient)
    double[][] TCMix = new double[n][n];
    double[][] PCMix = new double[n][n];
    double[][] nuMix = new double[n][n];
    for(int j=0;j<n;j++) {
      for(int k=0;k<n;k++) {
        TCMix[j][k] = Math.sqrt(TC[j] * TC[k]);
        PCMix[j][k] = (4*TCMix[j][k]) *
          ( ((PC[j]*VC[j])/TC[j]) + ((PC[k]*VC[k])/TC[k])
          ) /(Math.pow( (Math.pow(VC[j],tsq)+ Math.pow(VC[k],tsq)) , 3));
        nuMix[j][k] = 0.5*(nu[j]+nu[k]);
        double TR = mT/(TCMix[j][k]);
        double W = 0.5*(omegah[j]+omegah[k]);
        double muR = (Math.pow(10,5)*mu[j]*mu[k]*PCMix[j][k])
                  /(Math.pow(TCMix[j][k],2));
```

```
     double FB0 = (0.1445 - (0.330/TR) -
            (0.1385/Math.pow(TR, 2)) - (0.0121/Math.pow(TR, 3))
           );
     double FB1 = W * (0.073 + (0.46/TR) - (0.5/Math.pow(TR, 2)) -
              (0.097/Math.pow(TR, 3)) - (0.0073/Math.pow(TR, 8))
             );
     if(TR < 0.95 || muR >= 4) {
      double Fu = -5.237220 + (5.665807*Math.log(muR)) -
           (2.133816*Math.pow(Math.log(muR), 2)) +
           (0.2525373*Math.pow(Math.log(muR), 3)) +
           ((1/TR)*(5.769770-(6.181427*Math.log(muR)) +
            (2.283270*Math.pow(Math.log(muR), 2)) -
            (0.2649074*Math.pow(Math.log(muR),3)))
           );
      double Fa = (nuMix[j][k] * Math.exp(6.6*(0.7-TR)));
      Bv[j][k] = (FB0+FB1+Fu+Fa) * (82.057*TCMix[j][k]/PCMix[j][k]);
      Bv[k][j]= Bv[j][k];
     }
     else {
      Bv[j][k] =(  ((FB0+FB1)*82.057*TCMix[j][k])/PCMix[j][k] ) ;
      Bv[k][j] = Bv[j][k];
     }
    }  // end k
   } // end j
// Cal phi (fugacity coefficient)
   double port = P/(82.057*mT);
   double Bmix = 0;
   double sumy = 0;
   for(int j=0;j<n;j++) {
    for(int k=0;k<n;k++) {
     Bmix = Bmix + (y[i][j] * y[i][k] * Bv[j][k]);
    } // end k
   sumy = sumy + y[i][j];
   } // end j
```

```
      double sBmix = Bmix/Math.pow(sumy, 2);
      double sqarg = 0.25+sBmix*port;
      if(sqarg < 0) {
        double vmix = sBmix + (1/port);
        double zmix = port * vmix;
        sumy =0;
        for(int j=0;j<n;j++) {
          double sumb = 0;
          for(int k=0;k<n;k++) {
            sumb = sumb + y[i][k]*Bv[j][k];
          }
          sumy = sumy+ y[i][j];
          double sumbs = sumb/sumy;
          phi[i][j] = Math.exp(((2.0*sumbs)-sBmix)*port);
        }
      }
      else {
        double vmix = (0.5+Math.sqrt(sqarg))/port;
        double zmix = port*vmix;
        sumy = 0;
        for(int j=0;j<n;j++) {
          double sumb = 0;
          for(int k=0;k<n;k++) {
            sumb += y[i][k] * Bv[j][k];
          }
          sumy = sumy + y[i][j];
          double sumbs = sumb/sumy;
          phi[i][j] = Math.exp(2.0*sumbs/vmix)/zmix;
        }
      }
for(int j=0;j<n;j++) {
        K[i][j] = (gamma[i][j] * psat[i][j]) / (phi[i][j]*P);
      }
  };
```

```
  private void calX() {            // Calculation liquid composition by MESH equation
    for(int j=0;j<n;j++) {
      int i = 0;
      double tmpf= i>=f?F:0;
      double bx = -(V[i+1]+(tmpf-D)+D+(V[i]*K[i][j]));
      double cx = V[i+1] * K[i+1][j];
      double dx = 0;
      double p = cx/bx;
      double q = 0;
      x[i][j] = getX(i, j, p, q);
    }
// adjust x
    for(int i=0;i<m;i++) {
      double sumx = 0;
      for(int j=0;j<n;j++) {
        sumx = sumx+x[i][j];
      }
      if(sumx != 1) {
        for(int j=0;j<n;j++) {
          x[i][j] = x[i][j] / sumx;
        }
      }
    }
  };
private double getX(int i, int j, double p, double q) {
    if(i==0) {
      x[i][j] = q-(p*getX(i+1, j, p, q));
      return x[i][j];
    }
    else
    if(i>0 && i<m-1) {
      double tmpF= i-1>=f?F:0;
      double tmpf= i>=f?F:0;
```

```
    double ax = V[i] + tmpF - D;
    L[i] = V[i+1] + tmpf -D;
    double bx = -(V[i+1]+(tmpf-D)+(V[i]*K[i][j]));
    double cx = V[i+1] * K[i+1][j];
    double newp = cx/(bx-ax*p);
    double dx = i==f?-F*Z[j]:0;
    double newq = (dx - ax*q)/(bx- ax*p);
    x[i][j] = newq - (newp*getX(i+1, j, newp, newq));
    return x[i][j];
  }
  else
  if(i == m-1) {  // break here
    L[i]=B;
    double ax = V[i] + B;
    double bx = -((V[i]*K[i][j]) + B);
    double newq = (-ax*q)/(bx-ax*p);
    x[i][j] = newq;
    return x[i][j];
  }
  return 0;
};
```

```
  private void caly(){              // Calculate vapor composition
  for (int i=0;i<m;i++){
  for (int j=0; j<n;j++){
        y[i][j] = K[i][j]*x[i][j]; //calK at newT,new_x,init_y
  } //end i
  }// end j
//efficiency
  for (int i=1;i<m-1;i++){
    for (int j=0; j<n;j++){
        y[i][j] =( E[i]*(y[i][j]-y[i+1][j]) )+y[i+1][j];
    } //end i
    }// end j
//adjust y
  for(int i=0;i<m;i++){
   double sumy = 0;
   for(int j=0;j<n;j++){
   sumy = sumy+ y[i][j];
   } //end j
   if(sumy != 1) {
     for(int j=0;j<n;j++){
        y[i][j] = y[i][j] /sumy;
     }
   }
   }
  };
```

```
public void output() {          //Show Output forms
  DecimalFormat form1 = new DecimalFormat("#.###");
  MyDecimalFormat form2 = new MyDecimalFormat("####.###");
  form2.setMaximumIntegerDigits(4);
  _out.print("Stage ");
  for(int i=0;i<n;i++) {
    if(i+1 < 10)
      _out.print("  X"+(i+1)+"  ");
    else
      _out.print("  X"+(i+1)+" ");
  }
  for(int i=0;i<n;i++) {
    if(i+1 < 10)
      _out.print("  Y"+(i+1)+"  ");
    else
      _out.print("  Y"+(i+1)+" ");
  }
  _out.println("     V          L          T          Hv          Hl   ");
  for(int i=0;i<m;i++) {
    if(i+1 < 10)
      _out.print("  "+(i+1)+"   ");
    else
      _out.print(" "+(i+1)+"   ");
    for(int j=0;j<n;j++) {
      _out.print(form1.format(x[i][j])+" ");
    }
    for(int j=0;j<n;j++) {
      _out.print(form1.format(y[i][j])+" ");
    }
   _out.println(form2.myFormat(V[i])+" "+form2.myFormat(L[i])+" "+
                    form2.myFormat(T[i])+" "+form2.myFormat(Hv[i])+" "+
                    form2.myFormat(Hl[i]));
  }
  _out.flush();
```

```
 };
 public static void main(String args[ ]) { //call procedure in program
   Test t = new Test("infile", "outfile");
   t.process();
 };

 public void outputValue(double[ ][ ] a, String filename) {
   try {
     PrintWriter pw = new PrintWriter(new FileOutputStream(filename));
     for(int i=0;i<a.length;i++) {
       for(int j=0;j<a[0].length;j++) {
         pw.print(a[i][j]+" ");
       }
       pw.println(" ");
     }
     pw.flush();
   }catch(Exception e) {}
 };

public void outputValue(double[ ] a, String filename) {
   try {      PrintWriter pw = new PrintWriter(new FileOutputStream(filename));
     for(int i=0;i<a.length;i++) {
       pw.print(a[i] + " ");     }
     pw.flush();    }
catch(Exception e) {}
 };
};      // finish
```

Program for output pattern:

```
import java.text.*;
public class MyDecimalFormat extends DecimalFormat {
  public MyDecimalFormat(String format) {
    super(format);  };
  public String myFormat(double format) {
    if(format < 10) {
      applyPattern("'      '#.###");
    }
    else
    if(format < 100) {
      applyPattern("'     '##.###");
    }
    else
    if(format < 1000) {
      applyPattern("'    '###.###");
    }
    else
    if(format < 10000) {
      applyPattern("'   '####.###");
    }
    else
    if(format < 100000) {
      applyPattern("' '#####.###");
    }
    else
    if(format < 1000000) {
      applyPattern("######.###");
    }
    setMaximumIntegerDigits(6);
    setMinimumFractionDigits(3);
    setMaximumFractionDigits(3);
    return super.format(format);          };
};
```

Appendix B

Computer Program for Calculation Saturated Pressure

For ethanol :

```
import java.lang.*;
public class psat{   //for ethanol
public static void main (String args[]){
double a= -8.51838 ;
double b= 0.34163  ;
double c= -5.73683 ;
double d=  8.32581 ;
double TC= 513.9  ;
double PC= 61.4   ;
double []T ={ 241.85,261.15,270.85,281.15,292.15,299.15,308.05,321.55,336.65,
              351.55};
double []psat = new double [10];
      for(int j=0;j<10;j++) {
        double tao = 1 - (T[j] / TC);
        double logpsat = (1/(1-tao)) *
                         ( (a*tao) + (b*tao*Math.sqrt(tao)) +
                           (c*Math.pow(tao, 3)) + (d*Math.pow(tao, 6)) );
        psat[j] = (Math.exp(logpsat)) * PC ;
       System.out.println("T(K)= "+T[j]);
       System.out.println("Psat= "+psat[j]);
       }//end j
System.out.println("Saturated vapor pressure of ethanol by Wagner's equation.");
}
}
```

For water:

```
import java.lang.*;
public class psat1{   //water
public static void main (String args[]){
double a= -7.76451 ;
double b= 1.45838  ;
double c= -2.77580 ;
double d= -1.23303 ;
double TC= 647.3  ;
double PC= 221.2   ;
double []T ={ 273.15,283.15,293.15,303.15,313.15,323.15,333.15,343.15,
              353.15,363.15,373.15};
double []psat = new double [11];
      for(int j=0;j<11;j++) {
        double tao = 1 - (T[j] / TC);
        double logpsat = (1/(1-tao)) *
                         ( (a*tao) + (b*tao*Math.sqrt(tao)) +
                           (c*Math.pow(tao, 3)) + (d*Math.pow(tao, 6)) );
       psat[j] = (Math.exp(logpsat)) * PC ;
       System.out.println("T(K)= "+T[j]);
       System.out.println("Psat(bar)= "+psat[j]);
       }//end j
System.out.println("Saturated vapor pressure of water by Wagner's equation.");
}
}
```

Appendix C

Computer Program for Calculation Wilson parameter

```
import java.lang.*;
public class wilson { //  ethanol(1)+water(2) at 323.15 K
public static void main (String args[]){
double [] x ={0.0874,0.0967,0.1411,0.1756,0.2065,0.2253,0.2252,0.2856,0.3133,
            0.3535,0.3773,0.3999,0.4258,0.4691,0.4987,0.5218,0.5421,0.5692,
            0.5907,0.6242,0.6697,0.6868,0.7586,0.7811,0.8299,0.8454,0.8559,
            0.8638,0.8713,0.8801,0.8911,0.9031,0.9136,0.9263,0.9344,0.9480,
            0.9528 };  //ethanol
double [] g1={3.4513,3.3591,2.8214,2.4675,2.2331,2.0935,1.9235,1.7856,1.6845,
             1.5497,1.4861,1.4325,1.3738,1.2973,1.2495,1.2158,1.1950,1.1688,
             1.1436,1.1148,1.0817,1.0716,1.0366,1.0266,1.0129,1.0119,1.0090,
             1.0067,1.0067,1.0063,1.0057,1.0051,1.0039,1.0035,1.0014,1.0011,
             1.0001};  //ethanol
double [] g2={1.0187,1.0192,1.0463,1.0731,1.0995,1.1181,1.1505,1.1822,1.2124,
             1.2689,1.2967,1.3258,1.3637,1.4273,1.4825,1.5257,1.5551,1.5971,
             1.6439,1.7106,1.8037,1.8439,2.0159,2.0754,2.1990,2.2319,2.2551,
             2.2808,2.2856,2.2957,2.3121,2.3094,2.3544,2.3644,2.4221,2.4432,
             2.4777};   //water
double  A12, A21, A, B, R,a12,a21 ;
double Q1 = 0.1;
double Q2 = 0.1;
do{
A12=Q1;
A21=Q2;
double sum1 = 0;
double sum2 = 0;
double sum3 = 0;
double sum4 = 0;
double sum5 = 0;
```

```
      for (int i=0;i<37;i++){
         A = (x[i]*(1-x[i]))/((A12*(1-x[i]))+x[i]);
         sum1=sum1+ (Math.pow(A,2));
         B = (x[i]*(1-x[i]))/((1-x[i])+(A21*x[i]));
         sum2=sum2+ (Math.pow(B,2));
         sum3 = sum3+(A*B);
         R = ((x[i]*Math.log(g1[i]))+((1-x[i])*Math.log(g2[i])))
           +(x[i]*Math.log(x[i]+(A12*(1-x[i])))) +
           ((1-x[i])*Math.log((A21*x[i])+(1-x[i])));
         sum4 = sum4+(A*R);
         sum5 = sum5+(B*R);
      } //end i
         a12 = ((sum4*sum2)-(sum5*sum3))/((sum2*sum1)-(Math.pow(sum3,2)));
         a21 = (sum4-(sum1*(((sum4*sum2)-(sum5*sum3))/((sum2*sum1)-Math.pow(sum3,2)))))
               /sum3;
         Q1 = A12-a12;
         Q2 = A21-a21;
   }//end do
       while  ( Math.abs(a12) > 0.000001 && Math.abs(a21) >0.000001);
         System.out.println("T(K)= "+323.15);
         System.out.println("A12= "+Q1);
         System.out.println("A21= "+Q2);
}
}
```

Appendix D

Computer Program for Calculation Activity Coefficient

```
import java.lang.*;
public class para { //  ethanol(1)+water(2) at 323.15 K
public static void main (String args[]){
double [] x1 = {0.0874,0.0967,0.1411,0.1756,0.2065,0.2253,0.2252,0.2856,
                0.3133,0.3535,0.3773,0.3999,0.4258,0.4691,0.4987,0.5218,0.5421,
                0.5692,0.5907,0.6242,0.6697,0.6868,0.7586,0.7811,0.8299,0.8454,
                0.8559,0.8638,0.8713,0.8801,0.8911,0.9031,0.9136,0.9263,0.9344,
                0.9480,0.9528 };  //ethanol
double [] g1 = {3.4513,3.3591,2.8214,2.4675,2.2331,2.0935,1.9235,1.7856,1.6845,
                1.5497,1.4861,1.4325,1.3738,1.2973,1.2495,1.2158,1.1950,1.1688,
                1.1436,1.1148,1.0817,1.0716,1.0366,1.0266,1.0129,1.0119,1.0090,
                1.0067,1.0067,1.0063,1.0057,1.0051,1.0039,1.0035,1.0014,1.0011,
                1.0001};  //ethanol
double [] g2 = {1.0187,1.0192,1.0463,1.0731,1.0995,1.1181,1.1505,1.1822,1.2124,
                1.2689,1.2967,1.3258,1.3637,1.4273,1.4825,1.5257,1.5551,1.5971,
                1.6439,1.7106,1.8037,1.8439,2.0159,2.0754,2.1990,2.2319,2.2551,
                2.2808,2.2856,2.2957,2.3121,2.3094,2.3544,2.3644,2.4221,2.4432,
                2.4777};   //water
double T=323.15;
double  A21= ((0.001933167*T)+0.2035)*(1.45);
double  A12= ((-0.00087525*T)+0.477);
double [] gamma1=new double[37];
double [] gamma2=new double[37];
for(int i=0;i<37;i++){
gamma1[i]=(Math.exp((1-x1[i])*((A12/(x1[i]+(A12*(1-x1[i]))))-(A21/
          ((A21*x1[i])+(1-x1[i]))))))/(x1[i]+(A12*(1-x1[i])));
gamma2[i]=(Math.exp(-x1[i]*((A12/(x1[i]+(A12*(1-x1[i]))))-
          (A21/((A21*x1[i])+(1-x1[i]))))))/((1-x1[i])+(A21*x1[i]));
      System.out.print("G1 ethanol= "+gamma1[i]);
      System.out.println("    G2 water= "+gamma2[i]);
}//end of I  } }
```

Appendix E

Computer Program for Calculation Fugacity Coefficient

```
import java.lang.*;
public class calphi {  //   ethanol(1)+water(2) isobaric
public static void main(String args[]){
int n=2;
int m=18;
double[][]  phi = new double[m][n];
double[][]   Bv = new double[n][n];
double[][]y=new double[m][n];
 y[0][0] =0.366;y[1][0] =0.448;y[2][0] =0.539;y[3][0] =0.582;
 y[4][0] =0.600;y[5][0] =0.605;y[6][0] =0.627;y[7][0] =0.666;
 y[8][0] =0.712;y[9][0] =0.759;y[10][0] =0.764;y[11][0] =0.818;
 y[12][0] =0.851;y[13][0] =0.854;y[14][0] =0.856;y[15][0] =0.886;
 y[16][0] =0.907;y[17][0] =0.920;
for(int i=0;i<m;i++){
y[i][1]=1-y[i][0];}
double P=1.015;
double[] T={362.19,359.26,356.33,354.89,354.46,354.41,353.59,352.85,
            352.16,351.74,351.70,351.41,351.37,351.37,351.36,351.34,
            351.33,351.33};
double[]Z = new double[n];
    Z[1]  = 0.771;  Z[0] = 0.229;
double[]  TC  = new double[n];
   TC[1] = 647.3; TC[0] = 513.9;
double[]    PC = new double[n];
   PC[1] =221.2; PC[0] = 61.4;
double[]    VC = new double[n];
    VC[1] = 57.1; VC[0] = 167.1;
double[]    nu = new double[n];
    nu[1] = 0; nu[0] = 1.10;
```

```
double[]    omegah = new double[n];
    omegah[1] = 0.01; omegah[0] = 0.152;
double[]    mu = new double[n];
    mu[1] = 1.83; mu[0] = 1.69;
double[]  omega = new double[n];
    omega[1] = 0.344; omega[0] = 0.644;
double tsq= (1.0/3.0);
for(int i=0;i<m;i++){
// Cal B (second virial coefficient)
      double[][] TCMix = new double[n][n];
      double[][] PCMix = new double[n][n];
      double[][] nuMix = new double[n][n];
      for(int j=0;j<n;j++) {
        for(int k=0;k<n;k++) {
          TCMix[j][k] = Math.sqrt(TC[j] * TC[k]);
          PCMix[j][k] = (4*TCMix[j][k]) *
            ( ((PC[j]*VC[j])/TC[j]) + ((PC[k]*VC[k])/TC[k])
            ) /(Math.pow( (Math.pow(VC[j],tsq)+ Math.pow(VC[k],tsq)) , 3));
          nuMix[j][k] = 0.5*(nu[j]+nu[k]);
          double TR = T[i]/(TCMix[j][k]);
          double W = 0.5*(omegah[j]+omegah[k]);
          double muR = (Math.pow(10,5)*mu[j]*mu[k]*PCMix[j][k])
                      /(Math.pow(TCMix[j][k],2));
          double FB0 = (0.1445 - (0.330/TR) -
                        (0.1385/Math.pow(TR, 2)) - (0.0121/Math.pow(TR, 3))
                       );
          double FB1 = W * (0.073 + (0.46/TR) - (0.5/Math.pow(TR, 2)) -
                          (0.097/Math.pow(TR, 3)) - (0.0073/Math.pow(TR, 8))
                         );
          if(TR < 0.95 || muR >= 4) {
            double Fu = -5.237220 + (5.665807*Math.log(muR)) -
                      (2.133816*Math.pow(Math.log(muR), 2)) +
                      (0.2525373*Math.pow(Math.log(muR), 3)) +
                      ((1/TR)*(5.769770-(6.181427*Math.log(muR)) +
```

```
                    (2.283270*Math.pow(Math.log(muR), 2)) -
                    (0.2649074*Math.pow(Math.log(muR),3)))
                   );
            double Fa = (nuMix[j][k] * Math.exp(6.6*(0.7-TR)));
            Bv[j][k] = (FB0+FB1+Fu+Fa) * (82.057*TCMix[j][k]/PCMix[j][k]);
            Bv[k][j]= Bv[j][k];
          }
          else {
            Bv[j][k] =(  ((FB0+FB1)*82.057*TCMix[j][k])/PCMix[j][k] ) ;
            Bv[k][j] = Bv[j][k];
          }
        }  // end k
      } // end j
// Cal phi (fugacity coefficient)
      double port = P/(82.057*T[i]);
      double Bmix = 0;
      double sumy = 0;
      for(int j=0;j<n;j++) {
        for(int k=0;k<n;k++) {
          Bmix = Bmix + (y[i][j] * y[i][k] * Bv[j][k]);
        } // end k
      sumy = sumy + y[i][j];
      } // end j
      double sBmix = Bmix/Math.pow(sumy, 2);
      double sqarg = 0.25+sBmix*port;
      if(sqarg < 0) {
        double vmix = sBmix + (1/port);
        double zmix = port * vmix;
        sumy =0;
        for(int j=0;j<n;j++) {
          double sumb = 0;
          for(int k=0;k<n;k++) {
            sumb = sumb + y[i][k]*Bv[j][k];
          }
```

```
          sumy = sumy+ y[i][j];
          double sumbs = sumb/sumy;
          phi[i][j] = Math.exp(((2.0*sumbs)-sBmix)*port);
        }
      }
      else {
        double vmix = (0.5+Math.sqrt(sqarg))/port;
        double zmix = port*vmix;
        sumy = 0;
        for(int j=0;j<n;j++) {
          double sumb = 0;
          for(int k=0;k<n;k++) {
            sumb += y[i][k] * Bv[j][k];
          }
          sumy = sumy + y[i][j];
          double sumbs = sumb/sumy;
          phi[i][j] = Math.exp(2.0*sumbs/vmix)/zmix;
        }
      }
          System.out.println("phi1="+phi[i][0]);
          System.out.println("phi2="+phi[i][1]);
          }//end i
}
}
```

Appendix F

Computer Program for Calculation Enthalpy

For liquid phase:

```
import java.text.*;
import java.io.*;
public class heat01{
public static void main(String args[]){
    double R = 8.31451;//joules/mole.K
    int m=4;
    int n=2;
    int p=3;
    double[][]x = new double[m][n];
    for (int i=0;i<m;i++){
        x[0][0] = 0.2;                    x[0][1] = 0.8;
        x[1][0] = 0.4;                    x[1][1] = 0.4;
        x[2][0] = 0.6;                    x[2][1] = 0.6;
        x[3][0] = 0.8;                    x[3][1] = 0.2;
    }
   double  T[] = new double[p];
   T[0]=300; T[1]=330;  T[2]=360;
   double[] TC  = new double[n];
    TC[0] = 647.3; TC[1] = 513.9;
   double[] PC = new double[n];
    PC[0] = 221.2; PC[1] = 61.4;
   double[] VC = new double[n];
    VC[0] = 57.1; VC[1] = 167.1;
   double[] nu = new double[n];
    nu[0] = 0; nu[1] = 1.10;
  double[]  omegah = new double[n];
    omegah[0] = 0.01; omegah[1] = 0.152;
  double[]  mu = new double[n];
    mu[0] = 1.83; mu[1] = 1.69;
```

```
double[]  d1 = new double[n];
   d1[0] = 25.573; d1[1] = -744.60;
double[]  d2 = new double[n];
   d2[0] = 897.86; d2[1] = 21117;
double[] d3 = new double[n];
   d3[0] = 0.013705; d3[1] = -0.046915;
double[] d4 = new double[n];
   d4[0] = 0.15825; d4[1] = 132.08;
double[] c2 = new double[n];
   c2[0] = -7004.8; c2[1] = -3465.9;
double[] c3 = new double[n];
   c3[0] = 0.0035888; c3[1] = -0.062301;
double[] c4 = new double[n];
   c4[0] = -6.6689; c4[1] = 20.468;
double[] c5 = new double[n];
   c5[0] = -0.00000085054; c5[1] = 0.000020664;
double[] omega = new double[n];
  omega[0] = 0.344; omega[1] = 0.637;
  double P =1.013;//bar
  double T0=273.15;
  double[] Hv=new double[m];
  double[] Hl=new double[m];
 for(int k=0;k<p;k++){
           for(int i=0;i<m;i++) {
     System.out.println("T="+T[k]);
     //cal Hl
     double suml1=0;
     double suml2=0;
         for(int j=0;j<n;j++) {
  suml1 = suml1 + x[i][j] * ( (0.96*d1[j]*(T[k] - T0)) + (d2[j]*Math.log(T[k]/T0)) +
          (d3[j]*(Math.pow(T[k], 2)- Math.pow(T0, 2))/2) + (d4[j]*(T[k]*Math.log(T[k]) –
          (T0*Math.log(T0)) + T0 - T[k])) );
  suml2 = suml2 + x[i][j] * ( (-c2[j]) + (c3[j]*Math.pow(T[k], 2)) +
          (c4[j]*T[k]) + (2*c5[j]*Math.pow(T[k], 3))  );
```

```
   } //end j
 double lamda12 = (4.8515167*T[k])+2092.03;
 double lamda21 = (18.736775*T[k]) -4822.41;
 double a12 = 0.001933167*T[k] + 0.2035;
 double a21 = -0.00087525*T[k] +0.477;
  double he = x[i][0] * x[i][1] *
              ( ((lamda12*a12)/(x[i][0]+(a12*x[i][1]))) +
                ((lamda21*a21)/((a21*x[i][0]) + x[i][1]))     );
//cal Hlo
    double sumlo1=0;
    double sumlo2=0;
  for(int j=0;j<n;j++) {
  sumlo1 = sumlo1 + x[i][j] *
          ( (0.96*d1[j]*(273.15 - T0)) + (d2[j]*Math.log(273.15/T0)) +
            (d3[j]*(Math.pow(273.15, 2)- Math.pow(T0, 2))/2) +
            (d4[j]*(273.15*Math.log(273.15) - (T0*Math.log(T0)) + T0 - 273.15)) );
  sumlo2 = sumlo2 + x[i][j] *
          ( (-c2[j]) + (c3[j]*Math.pow(273.15, 2)) +
            (c4[j]*273.15) + (2*c5[j]*Math.pow(273.15, 3)) );
   } //end j
  double  lamdao12 = (4.8515167*273.15)+2092.03;
  double  lamdao21 = (18.736775*273.15) -4822.41;
  double  ao12 = 0.001933167*273.15 + 0.2035;
  double  ao21 = -0.00087525*273.15 +0.477;
  double heo = x[i][0] * x[i][1] *
              ( ((lamdao12*ao12)/(x[i][0]+(ao12*x[i][1]))) +
                ((lamdao21*ao21)/((ao21*x[i][0]) + x[i][1]))  );
  double Hlo = (( sumlo1 - R*sumlo2 +heo ) /1000);
    Hl[i] = (( suml1 - R*suml2 +he ) /1000)-Hlo ;//kJ/mol
     System.out.println("Hl[i]="+Hl[i]);
   } // end for i
}//endk
  }
  }
```

For vapor phase:

```
import java.text.*;
import java.io.*;
public class heat{
public static void main(String args[]){ //
    double R = 8.31451;//joules/mole.K
    int m=12;
    int n=2;
    double[][]x = new double[m][n]; //ethanol
    for (int i=0;i<m;i++){
        x[0][0] = 0.9;                x[0][1] = 0.1;
        x[1][0] = 0.95;               x[1][1] = 0.05;
        x[2][0] = 0.77;               x[2][1] = 0.23;
        x[3][0] = 0.60;               x[3][1] = 0.40;
        x[4][0] = 0.43;               x[4][1] = 0.57;
        x[5][0] = 0.30;               x[5][1] = 0.70;
        x[6][0] = 0.20;               x[6][1] = 0.80;
        x[7][0] = 0.10;               x[7][1] = 0.90;
        x[8][0] = 0.05;               x[8][1] = 0.95;
        x[9][0] = 0.03;               x[9][1] = 0.97;
        x[10][0] =0.03;                x[10][1] = 0.97;
        x[11][0] =0.01;                x[11][1] = 0.99;
    }
   double[][] y = new double[m][n];
   for(int i=0;i<m;i++){
        y[0][0] = 0.89;             y[0][1] = 0.11;
        y[1][0] = 0.94;             y[1][1] = 0.06;
        y[2][0] = 0.79;             y[2][1] = 0.21;
        y[3][0] = 0.68;             y[3][1] = 0.32;
        y[4][0] = 0.62;             y[4][1] = 0.38;
        y[5][0] = 0.58;             y[5][1] = 0.42;
        y[6][0] = 0.52;             y[6][1] = 0.48;
        y[7][0] = 0.41;             y[7][1] = 0.59;
        y[8][0] = 0.33;             y[8][1] = 0.67;
```

```
     y[9][0] = 0.24;                  y[9][1] = 0.76;
     y[10][0] = 0.18;                 y[10][1] = 0.82;
     y[11][0] = 0.10;                 y[11][1] = 0.90;
      }
 double[]  T = {351.3,351.4,351.5,352.3,353.5,354.7,356.3,
               360.3,363.7,366.5,368.3,370.4};
 double[] TC  = new double[n];
  TC[1] = 647.3; TC[0] = 513.9;
 double[] PC = new double[n];
  PC[1] = 221.14; PC[0] = 61.4;
 double[] VC = new double[n];
  VC[1] = 57.1; VC[0] = 167.1;
 double[] nu = new double[n];
  nu[1] = 0; nu[0] = 1.10;
double[]  omegah = new double[n];
  omegah[1] = 0.01; omegah[0] = 0.152;
double[]  mu = new double[n];
  mu[1] = 1.83; mu[0] = 1.69;
double[]  d1 = new double[n];
  d1[1] = 25.573; d1[0] = -744.60;
double[]  d2 = new double[n];
  d2[1] = 897.86; d2[0] = 21117;
 double[] d3 = new double[n];
  d3[1] = 0.013705; d3[0] = -0.046915;
 double[] d4 = new double[n];
  d4[1] = 0.15825; d4[0] = 132.08;
 double[] c2 = new double[n];
  c2[1] = -7004.8; c2[0] = -3465.9;
 double[] c3 = new double[n];
  c3[1] = 0.0035888; c3[0] = -0.062301;

 double[] c4 = new double[n];
  c4[1] = -6.6689; c4[0] = 20.468;
 double[] c5 = new double[n];
```

```
   c5[1] = -0.00000085054; c5[0] = 0.000020664;
 double[] omega = new double[n];
   omega[1] = 0.344; omega[0] = 0.637;
double P =1.013;//bar
double T0=273.15;
double[] Hv=new double[m];
double[] Hl=new double[m];
double[] lamda12 = new double[m];
double[] lamda21 = new double[m];
double[] a12 = new double[m];
double[] a21 = new double[m];
 for(int i=0;i<m;i++) {
     //cal Hl
     double suml1=0;
     double suml2=0;
  for(int j=0;j<n;j++) {
  suml1 = suml1 + x[i][j] *
         ( (0.96*d1[j]*(T[i] - T0)) + (d2[j]*Math.log(T[i]/T0)) +
           (d3[j]*(Math.pow(T[i], 2)- Math.pow(T0, 2))/2) +
           (d4[j]*(T[i]*Math.log(T[i]) - (T0*Math.log(T0)) + T0 - T[i]))
         );
  suml2 = suml2 + x[i][j] *
         ( (-c2[j]) + (c3[j]*Math.pow(T[i], 2)) +
           (c4[j]*T[i]) + (2*c5[j]*Math.pow(T[i], 3))
         );
   } //end j
  lamda21[i] = (4.8515167*T[i])+2092.03;
  lamda12[i] = (18.736775*T[i]) -4822.41;
  a21[i] = 0.001933167*T[i] + 0.2035;
  a12[i] = -0.00087525*T[i] +0.477;

  double he = x[i][0] * x[i][1] *
            ( ((lamda12[i]*a12[i])/(x[i][0]+(a12[i]*x[i][1]))) +
             ((lamda21[i]*a21[i])/((a21[i]*x[i][0]) + x[i][1]))
```

```
              );
 // cal Hlo
      double sumlo1=0;
      double sumlo2=0;
   for(int j=0;j<n;j++) {
   sumlo1 = sumlo1 + x[i][j] *
           ( (0.96*d1[j]*(273.15 - T0)) + (d2[j]*Math.log(273.15/T0)) +
             (d3[j]*(Math.pow(273.15, 2)- Math.pow(T0, 2))/2) +
             (d4[j]*(273.15*Math.log(273.15) - (T0*Math.log(T0)) + T0 - 273.15))
           );
   sumlo2 = sumlo2 + x[i][j] *
           ( (-c2[j]) + (c3[j]*Math.pow(273.15, 2)) +
             (c4[j]*273.15) + (2*c5[j]*Math.pow(273.15, 3))
           );
   } //end j
   double  lamdao21 = (4.8515167*273.15)+2092.03;
   double  lamdao12 = (18.736775*273.15) -4822.41;
   double  ao21 = 0.001933167*273.15 + 0.2035;
   double  ao12 = -0.00087525*273.15 +0.477;
   double heo = x[i][0] * x[i][1] *
               ( ((lamdao12*ao12)/(x[i][0]+(ao12*x[i][1]))) +
                 ((lamdao21*ao21)/((ao21*x[i][0]) + x[i][1]))
               );
   double Hlo = ( sumlo1 - R*sumlo2 +heo )/1000 ;
   Hl[i] = ( (suml1 - R*suml2 +he )/1000 )-Hlo ;//kJ/mol
   System.out.println("T="+T[i]);
// cal Hv
      double sumv1 = 0;
      double sumv2 = 0;
      double[] TR = new double[n];

   for(int j=0;j<n;j++) {
        TR[j]=T[i]/TC[j];
   sumv1 = sumv1 + y[i][j] *
```

```
          ( (0.96*d1[j]*(T[i] - T0)) + (d2[j]*Math.log(T[i]/T0)) +
            (d3[j]*(Math.pow(T[i], 2)- Math.pow(T0, 2))/2) +
            (d4[j]*(T[i]*Math.log(T[i]) - (T0*Math.log(T0)) + T0 - T[i]))
          );
    sumv2 = sumv2 + (TC[j]*(P/PC[j]))*(-(0.1445+(0.073*omega[j]))+
          ((0.660-(0.92*omega[j]))/TR[j])+((0.4155+(1.50*omega[j]))/
           Math.pow(TR[j],2))+((0.0484+(0.388*omega[j]))/Math.pow(TR[j],3))
           + ((0.0657*omega[j])/Math.pow(TR[j],8))
           );
    } //end j
   double latent =( (x[i][0]*(R*4300))+(x[i][1]*(R*4400)) )/1000;
    Hv[i] = (( sumv1-R*sumv2 )/1000)+ latent + Hl[i] ;  //kJ/mol
    System.out.println("Hv[i]="+Hv[i]);
     } // end for i
}
}
```

APPENDIX G

Results

Table5.1 Saturated pressure of ethanol from Wagner's equation and experiment.

Number	Temperature(K)	$Psat_{exp}$(bar)	$Psat_{cal}$(bar)	$\lvert(Psat_{cal}-Psat_{exp})/Psat_{exp}\rvert$
1	241.85	0.001333	0.001354	0.015753938
2	261.15	0.006666	0.006695	0.004350435
3	270.85	0.013332	0.013697	0.027377738
4	281.15	0.026664	0.027680	0.038103810
5	292.15	0.053329	0.055344	0.037784320
6	299.15	0.079993	0.083566	0.044666408
7	308.05	0.133332	0.136953	0.027156231
8	321.55	0.266645	0.273237	0.024722009
9	336.65	0.533289	0.548861	0.029199927
10	351.55	1.013250	1.020080	0.006740686
Sum of data		2.127833	2.167467	0.255855503

N= number of data points

%Average Absolute Deviation = $\frac{1}{N}\left[\sum_{N}\left|\frac{P_{cal}^{sat}-P_{exp}^{sat}}{P_{exp}^{sat}}\right|\right]x100$

= (0.255855503x100)/10

= 2.56%

Table5.2 Saturated pressure of water from Wagner's equation and experiment.

Number	Temperature(K)	$Psat_{exp}$(bar)	$Psat_{cal}$(bar)	$\lvert(Psat_{cal}-Psat_{exp})/Psat_{exp}\rvert$
1	273.15	0.006104	0.006115	0.00180210
2	283.15	0.012277	0.012289	0.00097744
3	293.15	0.023378	0.023406	0.00119771
4	303.15	0.042428	0.042485	0.00134345
5	313.15	0.073737	0.073859	0.00165453
6	323.15	0.123336	0.123507	0.00138646
7	333.15	0.199156	0.199406	0.00125530
8	343.15	0.311574	0.311877	0.00097248
9	353.15	0.473427	0.473915	0.00103078
10	363.15	0.700955	0.701487	0.00075896
11	373.15	1.013250	1.013782	0.00052504
Sum of data		2.979622	2.982128	0.01290425

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\frac{P_{cal}^{sat}-P_{exp}^{sat}}{P_{exp}^{sat}}\right|\right]x100$$

$$= (0.01290425x100)/11$$

$$= 0.12\%$$

Table5.3 Activity coefficient of ethanol from Wilson equation and experiment at323.15K.

Number	Mole fraction (x_1)	Activity coefficient (γ_{exp})	Activity coefficient (γ_{cal})	$\lvert(\gamma_{cal} - \gamma_{exp})/ \gamma_{exp} \rvert$
1	0.0874	3.4513	3.42775	0.0068235
2	0.0967	3.3591	3.27225	0.0258551
3	0.1411	2.8214	2.69327	0.0454136
4	0.1756	2.4675	2.37379	0.0379777
5	0.2065	2.2331	2.15117	0.0366889
6	0.2253	2.0935	2.03770	0.0266539
7	0.2252	1.9235	2.03826	0.0596621
8	0.2856	1.7856	1.75418	0.0175963
9	0.3133	1.6845	1.65445	0.0178391
10	0.3535	1.5497	1.53417	0.0100213
11	0.3773	1.4861	1.47397	0.0081623
12	0.3999	1.4325	1.42304	0.0066038
13	0.4258	1.3738	1.37113	0.0019435
14	0.4691	1.2973	1.29722	0.0000616
15	0.4987	1.2495	1.25442	0.0039376
16	0.5218	1.2158	1.22472	0.0073367
17	0.5421	1.1950	1.20100	0.0050209
18	0.5692	1.1688	1.17240	0.0030801
19	0.5907	1.1436	1.15204	0.0073802
20	0.6242	1.1148	1.12385	0.0081180

Table5.3 (continued)

Number	Mole fraction (x_1)	Activity coefficient (γ_{exp})	Activity coefficient (γ_{cal})	$\vert(\gamma_{cal} - \gamma_{exp})/\gamma_{exp}\vert$
21	0.6697	1.0817	1.09171	0.0092540
22	0.6868	1.0716	1.08125	0.0090052
23	0.7586	1.0366	1.04564	0.0087208
24	0.7811	1.0266	1.03694	0.0100721
25	0.8299	1.0129	1.02162	0.0086089
26	0.8454	1.0119	1.01770	0.0057318
27	0.8559	1.0090	1.01528	0.0062240
28	0.8638	1.0067	1.01359	0.0068441
29	0.8713	1.0067	1.01209	0.0053541
30	0.8801	1.0063	1.01044	0.0041141
31	0.8911	1.0057	1.00856	0.0028438
32	0.9031	1.0051	1.00674	0.0016317
33	0.9136	1.0039	1.00533	0.0014244
34	0.9263	1.0035	1.00385	0.0003488
35	0.9344	1.0014	1.00304	0.0016377
36	0.9480	1.0011	1.0019	0.0007991
37	0.9528	1.0001	1.0015	0.0013999
Sum of data		53.3372	53.00796	0.4201911

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\frac{\gamma_{cal} - \gamma_{exp}}{\gamma_{exp}}\right|\right]\text{x}100$$

$$= (0.4201911\text{x}100)/37$$

$$= 1.14\%$$

Table5.4 Activity coefficient of water from Wilson equation and experiment at 323.15K.

Number	Mole fraction (x_1)	Activity coefficient (γ_{exp})	Activity coefficient (γ_{cal})	$\|(\gamma_{cal} - \gamma_{exp})/ \gamma_{exp}\|$
1	0.9126	1.0187	1.02478	0.0059684
2	0.9033	1.0192	1.02961	0.0102139
3	0.8589	1.0463	1.05687	0.0101023
4	0.8244	1.0731	1.08222	0.0084987
5	0.7935	1.0995	1.10764	0.0074034
6	0.7747	1.1181	1.12429	0.0055362
7	0.7748	1.1505	1.12419	0.0228683
8	0.7144	1.1822	1.18336	0.0009812
9	0.6867	1.2124	1.21332	0.0007588
10	0.6465	1.2689	1.25994	0.0070612
11	0.6227	1.2967	1.28931	0.0056991
12	0.6001	1.3258	1.31844	0.0055514
13	0.5742	1.3637	1.35333	0.0076043
14	0.5309	1.4273	1.41538	0.0083514
15	0.5013	1.4825	1.46059	0.0147791
16	0.4782	1.5257	1.4975	0.0184833
17	0.4579	1.5551	1.53116	0.0153945
18	0.4308	1.5971	1.57795	0.0119905
19	0.4093	1.6439	1.61662	0.0165947
20	0.3758	1.7106	1.67976	0.0180288
21	0.3303	1.8037	1.77143	0.0178910
22	0.3132	1.8439	1.80775	0.0196052
23	0.2414	2.0159	1.97229	0.0216330
24	0.2189	2.0754	2.02814	0.0227715

Table5.4 (continued)

Number	Mole fraction (x_1)	Activity coefficient (γ_{exp})	Activity coefficient (γ_{cal})	$\lvert(\gamma_{cal} - \gamma_{exp})/\gamma_{exp}\rvert$
25	0.1701	2.1990	2.15697	0.0191132
26	0.1546	2.2319	2.20022	0.0141942
27	0.1441	2.2551	2.23018	0.0110505
28	0.1362	2.2808	2.25310	0.0121449
29	0.1287	2.2856	2.27515	0.0045721
30	0.1199	2.2957	2.30130	0.0024393
31	0.1089	2.3121	2.33476	0.0098006
32	0.0969	2.3094	2.37192	0.0270720
33	0.0864	2.3544	2.40508	0.0215257
34	0.0737	2.3644	2.44603	0.0345246
35	0.0656	2.4221	2.47263	0.0208621
36	0.052	2.4432	2.51817	0.0306852
37	0.0472	2.4777	2.53415	0.0227832
Sum of data		64.0876	64.02553	0.5145377

N= number of data points

%Average Absolute Deviation = $\frac{1}{N}\left[\sum_{N}\left|\frac{\gamma_{cal}-\gamma_{exp}}{\gamma_{exp}}\right|\right]$x100

= (0.5145377x100)/37

= 1.39%

Table5.5 The calculation fugacity coefficient data of ethanol(1)+water(2).

T(K)	x_1	y_1	$\hat{\phi}_1$	$\hat{\phi}_2$
362.19	0.056	0.366	1.034919	0.982358
359.26	0.091	0.448	1.03409	0.982190
356.33	0.189	0.539	1.03259	0.982112
354.89	0.286	0.582	1.03183	0.982085
354.46	0.323	0.600	1.031381	0.982108
354.41	0.331	0.605	1.03121	0.982127
353.59	0.419	0.627	1.030843	0.982106
352.85	0.512	0.666	1.029715	0.982205
352.16	0.620	0.712	1.028263	0.982370
351.74	0.704	0.759	1.02662	0.982608
351.70	0.715	0.764	1.026444	0.982635
351.41	0.798	0.818	1.024481	0.982968
351.37	0.843	0.851	1.023233	0.983209
351.37	0.847	0.854	1.023119	0.983232
351.36	0.849	0.856	1.023048	0.983246
351.34	0.884	0.886	1.021925	0.983477
351.33	0.908	0.907	1.021146	0.983644
351.33	0.922	0.920	1.020665	0.983750

Table5.6 Enthalpy of ethanol(1)+water(2) liquid mixture from Eq.(3-110)and experiment.

Number	Mole fraction (x_1)	Temperature (K)	Enthalpy (HI_{exp})	Enthalpy (HI_{cal})	$\lvert(HI_{cal}-HI_{exp})/HI_{exp}\rvert$
1	0.2	300	2.25	2.270	0.008888889
2	0.2	330	4.9	4.880	0.004081633
3	0.2	360	7.5	7.550	0.006666667
4	0.4	300	2.5	2.450	0.020000000
5	0.4	330	5.4	5.350	0.009259259
6	0.4	360	8.5	8.420	0.009411765
7	0.6	300	2.7	2.590	0.040740741
8	0.6	330	5.7	5.750	0.008771930
9	0.6	360	8.8	9.180	0.043181818
10	0.8	300	2.7	2.710	0.003703704
11	0.8	330	6.0	6.110	0.018333333
12	0.8	360	9.0	9.877	0.097444444
Sum of data			65.95	67.137	0.270484182

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\frac{HI_{cal} - HI_{exp}}{HI_{exp}}\right|\right]x100$$

$$= (0.270484182x100)/12$$

$$= 2.25\%$$

Table5.7 Enthalpy of ethanol(1)+water(2) vapor mixture from Eq.(3-100)and experiment.

Number	Temperature (K)	Mole fraction (x_1)	Enthalpy (Hv_{exp})	Enthalpy (Hv_{cal})	$\lvert(Hv_{cal}-Hv_{exp})/Hv_{exp}\rvert$
1	351.3	0.89	47.5	44.25	0.068421053
2	351.4	0.95	47.5	48.76	0.026526316
3	351.5	0.77	47.5	48.17	0.014105263
4	352.3	0.6	47.5	47.81	0.006526316
5	353.5	0.43	47.5	47.58	0.001684211
6	354.7	0.3	47.5	47.4	0.002105263
7	356.3	0.2	47.6	47.24	0.007563025
8	360.3	0.1	47.6	47.18	0.008823529
9	363.7	0.05	47.8	47.19	0.012761506
10	366.5	0.03	47.8	47.17	0.013179916
11	368.3	0.03	48	47.19	0.016875000
12	370.4	0.01	48	47.06	0.019583333
Sum of data			571.8	567	0.198154732

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\frac{Hv_{cal}-Hv_{exp}}{Hv_{exp}}\right|\right]x100$$

$$= (0.198154732x100)/12$$

$$= 1.65\%$$

Table5.8 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = $1.05A_{21}$.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
1	0.0874	3.4513	3.3085	0.043161554	1.0187	1.0245	0.0056935
2	0.0967	3.3591	3.1603	0.062905420	1.0192	1.0293	0.0099097
3	0.1411	2.8214	2.6087	0.081534864	1.0463	1.0561	0.0093663
4	0.1756	2.4675	2.3043	0.070824111	1.0731	1.0810	0.0073618
5	0.2065	2.2331	2.0922	0.067345378	1.0995	1.1059	0.0058208
6	0.2253	2.0935	1.9841	0.055138350	1.1181	1.1221	0.0035775
7	0.2252	1.9235	1.9847	0.030835895	1.1505	1.1221	0.0246849
8	0.2856	1.7856	1.7142	0.041652083	1.1822	1.1797	0.0021147
9	0.3133	1.6845	1.6192	0.040328557	1.2124	1.2087	0.0030518
10	0.3535	1.5497	1.5048	0.029837852	1.2689	1.2538	0.0119001
11	0.3773	1.4861	1.4476	0.026595745	1.2967	1.2821	0.0112594
12	0.3999	1.4325	1.3992	0.023799314	1.3258	1.3101	0.0118419
13	0.4258	1.3738	1.3499	0.017705015	1.3637	1.3435	0.0148126
14	0.4691	1.2973	1.2798	0.013674012	1.4273	1.4028	0.0171653
15	0.4987	1.2495	1.2393	0.008230453	1.4825	1.4457	0.0248229
16	0.5218	1.2158	1.2110	0.003963666	1.5257	1.4807	0.0294947
17	0.5421	1.195	1.1887	0.005299907	1.5551	1.5125	0.0273937
18	0.5692	1.1688	1.1617	0.006111733	1.5971	1.5566	0.0253585
19	0.5907	1.1436	1.1425	0.000962801	1.6439	1.5929	0.0310238
20	0.6242	1.1148	1.1159	0.000985751	1.7106	1.6519	0.0343154
21	0.6697	1.0817	1.0856	0.003592483	1.8037	1.7372	0.0368687
22	0.6868	1.0716	1.0758	0.003904071	1.8439	1.7708	0.0396442
23	0.7586	1.0366	1.0424	0.005564083	2.0159	1.9220	0.0465797
24	0.7811	1.0266	1.0343	0.007444649	2.0754	1.9730	0.0493399
25	0.8299	1.0129	1.0200	0.006960784	2.199	2.0898	0.0496589

Table5.8 (continued).

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
26	0.8454	1.0119	1.0164	0.004427391	2.2319	2.1288	0.0461938
27	0.8559	1.0090	1.0141	0.005029090	2.2551	2.1557	0.0440779
28	0.8638	1.0067	1.0126	0.005826585	2.2808	2.1763	0.0458173
29	0.8713	1.0067	1.0112	0.004450158	2.2856	2.196	0.0392020
30	0.8801	1.0063	1.0096	0.003268621	2.2957	2.2195	0.0331925
31	0.8911	1.0057	1.0079	0.002182756	2.3121	2.2493	0.0271615
32	0.9031	1.0051	1.0062	0.001093222	2.3094	2.2825	0.0116480
33	0.9136	1.0039	1.0049	0.000995124	2.3544	2.3119	0.0180513
34	0.9263	1.0035	1.0036	0.000099641	2.3644	2.3483	0.0068093
35	0.9344	1.0014	1.0028	0.001396091	2.4221	2.3718	0.0207671
36	0.9480	1.0011	1.0017	0.000598982	2.4432	2.4121	0.0127292
37	0.9528	1.0001	1.0014	0.001298183	2.4777	2.4265	0.0206643
Sum of data		53.337	52.1671	0.689024375	64.0876	62.5335	0.8593751

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1\exp}}{\gamma_{1\exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2\exp}}{\gamma_{2\exp}}\right)\right|\right]x100$$

= ((0.689024375+0.8593571) x 100)/37

= 4.18%

Table5.9 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = 0.95A_{21}.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
1	0.0874	3.4513	3.5523	0.0292643	1.0187	1.0251	0.006283
2	0.0967	3.3591	3.3891	0.0089310	1.0192	1.0300	0.010597
3	0.1411	2.8214	2.7816	0.0141065	1.0463	1.0576	0.010800
4	0.1756	2.4675	2.4464	0.0085512	1.0731	1.0834	0.009598
5	0.2065	2.2331	2.2129	0.0090457	1.0995	1.1094	0.009004
6	0.2253	2.0935	2.0938	0.0001433	1.1181	1.1264	0.007423
7	0.2252	1.9235	2.0944	0.0888485	1.1505	1.1263	0.021034
8	0.2856	1.7856	1.7962	0.0059364	1.1822	1.1870	0.004060
9	0.3133	1.6845	1.6914	0.0040962	1.2124	1.2178	0.004454
10	0.3535	1.5497	1.5651	0.0099374	1.2689	1.2660	0.002285
11	0.3773	1.4861	1.5017	0.0104973	1.2967	1.2965	0.000154
12	0.3999	1.4325	1.4482	0.0109599	1.3258	1.3267	0.000679
13	0.4258	1.3738	1.3935	0.0143398	1.3637	1.3631	0.000440
14	0.4691	1.2973	1.3156	0.0141062	1.4273	1.4280	0.000490
15	0.4987	1.2495	1.2705	0.0168067	1.4825	1.4755	0.004722
16	0.5218	1.2158	1.2391	0.0191643	1.5257	1.5144	0.007406
17	0.5421	1.1950	1.2141	0.0159833	1.5551	1.5500	0.003280
18	0.5692	1.1688	1.1839	0.0129192	1.5971	1.5997	0.001628
19	0.5907	1.1436	1.1623	0.0163519	1.6439	1.6408	0.001886
20	0.6242	1.1148	1.1324	0.0157876	1.7106	1.7083	0.001345
21	0.6697	1.0817	1.0982	0.0152538	1.8037	1.8068	0.001719
22	0.6868	1.0716	1.0871	0.0144644	1.8439	1.8460	0.001139
23	0.7586	1.0366	1.0491	0.0120587	2.0159	2.0250	0.004514
24	0.7811	1.0266	1.0398	0.0128580	2.0754	2.0863	0.005252

Table5.9 (continued).

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
25	0.8299	1.0129	1.0234	0.0103663	2.1990	2.2285	0.013415
26	0.8454	1.0119	1.0191	0.0071153	2.2319	2.2765	0.019983
27	0.8559	1.0090	1.0165	0.0074331	2.2551	2.3099	0.024300
28	0.8638	1.0067	1.0147	0.0079468	2.2808	2.3355	0.023983
29	0.8713	1.0067	1.0131	0.0063574	2.2856	2.3601	0.032595
30	0.8801	1.0063	1.0113	0.0049687	2.2957	2.3894	0.040815
31	0.8911	1.0057	1.0093	0.0035796	2.3121	2.4269	0.049652
32	0.9031	1.0051	1.0073	0.0021888	2.3094	2.4686	0.068936
33	0.9136	1.0039	1.0058	0.0018926	2.3544	2.5060	0.064390
34	0.9263	1.0035	1.0042	0.0006976	2.3644	2.5522	0.079428
35	0.9344	1.0014	1.0033	0.0018973	2.4221	2.5823	0.066141
36	0.9480	1.0011	1.0021	0.0009989	2.4432	2.6340	0.078094
37	0.9528	1.0001	1.0017	0.0015998	2.4777	2.6526	0.070590
Sum of data		53.3372	53.8905	0.4374535	64.0876	65.6186	0.752515

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1exp}}{\gamma_{1exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2exp}}{\gamma_{2exp}}\right)\right|\right]x100$$

= ((0.4374535+0.752515) x 100)/37

= 3.22%

Table5.10 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = 1.10A_{21}.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert (\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert (\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
1	0.0874	3.4513	3.1942	0.0744937	1.0187	1.0242	0.005399
2	0.0967	3.3591	3.0531	0.0910958	1.0192	1.0289	0.009517
3	0.1411	2.8214	2.5278	0.1040618	1.0463	1.0553	0.008602
4	0.1756	2.4675	2.2379	0.0930496	1.0731	1.0797	0.006150
5	0.2065	2.2331	2.0359	0.0883077	1.0995	1.1041	0.004184
6	0.2253	2.0935	1.9330	0.0766659	1.1181	1.1199	0.001610
7	0.2252	1.9235	1.9335	0.0051989	1.1505	1.1199	0.026597
8	0.2856	1.7856	1.676	0.0613799	1.1822	1.1759	0.005329
9	0.3133	1.6845	1.5857	0.0586524	1.2124	1.2040	0.006928
10	0.3535	1.5497	1.4769	0.0469768	1.2689	1.2475	0.016865
11	0.3773	1.4861	1.4225	0.0427966	1.2967	1.2748	0.016889
12	0.3999	1.4325	1.3766	0.0390227	1.3258	1.3017	0.018178
13	0.4258	1.3738	1.3298	0.0320280	1.3637	1.3337	0.021999
14	0.4691	1.2973	1.2633	0.0262083	1.4273	1.3902	0.025993
15	0.4987	1.2495	1.2249	0.0196879	1.4825	1.4310	0.034739
16	0.5218	1.2158	1.1983	0.0143938	1.5257	1.4641	0.040375
17	0.5421	1.195	1.1771	0.0149791	1.5551	1.4941	0.039226
18	0.5692	1.1688	1.1516	0.0147159	1.5971	1.5356	0.038507
19	0.5907	1.1436	1.1334	0.0089192	1.6439	1.5696	0.045197
20	0.6242	1.1148	1.1084	0.0057409	1.7106	1.6248	0.050158
21	0.6697	1.0817	1.0799	0.0016640	1.8037	1.7046	0.054943
22	0.6868	1.0716	1.0707	0.0008399	1.8439	1.7352	0.058973
23	0.7586	1.0366	1.0394	0.0027011	2.0159	1.8741	0.070341
24	0.7811	1.0266	1.0319	0.0051627	2.0754	1.9260	0.071986

Table5.10 (continued).

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
25	0.8299	1.0129	1.0185	0.0055287	2.1990	2.0265	0.078445
26	0.8454	1.0119	1.0152	0.0032612	2.2319	2.0617	0.076258
27	0.8559	1.0090	1.0131	0.0040634	2.2551	2.0859	0.075030
28	0.8638	1.0067	1.0116	0.0048674	2.2808	2.1044	0.077341
29	0.8713	1.0067	1.0100	0.0032780	2.2856	2.1221	0.071535
30	0.8801	1.0063	1.0089	0.0025837	2.2957	2.1432	0.066429
31	0.8911	1.0057	1.0073	0.0015909	2.3121	2.1699	0.061503
32	0.9031	1.0051	1.0057	0.0005970	2.3094	2.1994	0.047631
33	0.9136	1.0039	1.0045	0.0005977	2.3544	2.2257	0.054664
34	0.9263	1.0035	1.0033	0.0001993	2.3644	2.2580	0.045001
35	0.9344	1.0014	1.0026	0.0011983	2.4221	2.2789	0.059122
36	0.9480	1.0011	1.0016	0.0004995	2.4432	2.3145	0.052677
37	0.9528	1.0001	1.0013	0.0011999	2.4777	2.3273	0.060701
Sum of data		53.3372	51.3654	0.9582076	64.0876	61.1363	1.505021

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1\exp}}{\gamma_{1\exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2\exp}}{\gamma_{2\exp}}\right)\right|\right]\text{x}100$$

= ((0.9582076+1.505021) x 100)/37

= 6.66%

Table5.11 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = $0.90A_{21}$.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
1	0.0874	3.4513	3.6823	0.0669313	1.0187	1.0253	0.006479
2	0.0967	3.3591	3.5111	0.0452502	1.0192	1.0303	0.010891
3	0.1411	2.8214	2.874	0.0186432	1.0463	1.0583	0.011469
4	0.1756	2.4675	2.5225	0.0222898	1.0731	1.0846	0.010717
5	0.2065	2.2331	2.2775	0.0198827	1.0995	1.1110	0.010459
6	0.2253	2.0935	2.1526	0.0282302	1.1181	1.1284	0.009212
7	0.2252	1.9235	2.1532	0.1194177	1.1505	1.1283	0.019296
8	0.2856	1.7856	1.8403	0.0306340	1.1822	1.1905	0.007021
9	0.3133	1.6845	1.7303	0.0271891	1.2124	1.2223	0.008166
10	0.3535	1.5497	1.5976	0.0309092	1.2689	1.2720	0.002443
11	0.3773	1.4861	1.5310	0.0302133	1.2967	1.3035	0.005244
12	0.3999	1.4325	1.4747	0.0294590	1.3258	1.3350	0.006939
13	0.4258	1.3738	1.4172	0.0315912	1.3637	1.3728	0.006673
14	0.4691	1.2973	1.3352	0.0292145	1.4273	1.4407	0.009388
15	0.4987	1.2495	1.2876	0.0304922	1.4825	1.4905	0.005396
16	0.5218	1.2158	1.2545	0.0318309	1.5257	1.5315	0.003802
17	0.5421	1.1950	1.2280	0.0276151	1.5551	1.5691	0.009003
18	0.5692	1.1688	1.1960	0.0232717	1.5971	1.6217	0.015403
19	0.5907	1.1436	1.1732	0.0258832	1.6439	1.6655	0.013139
20	0.6242	1.1148	1.1415	0.0239505	1.7106	1.7375	0.015725
21	0.6697	1.0817	1.1052	0.0217251	1.8037	1.8433	0.021955
22	0.6868	1.0716	1.0934	0.0203434	1.8439	1.8856	0.022615
23	0.7586	1.0366	1.0529	0.0157245	2.0159	2.0804	0.031996
24	0.7811	1.0266	1.0429	0.0158777	2.0754	2.1476	0.034788

Table5.11 (continued).

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert (\gamma_{1cal} - \gamma_{1exp}) / \gamma_{1exp} \rvert$	γ_{2exp}	γ_{2exp}	$\lvert (\gamma_{2cal} - \gamma_{2exp}) / \gamma_{2exp} \rvert$
25	0.8299	1.0129	1.0253	0.0122421	2.1990	2.3048	0.048113
26	0.8454	1.0119	1.0207	0.0086965	2.2319	2.3582	0.056589
27	0.8559	1.0090	1.018	0.0089197	2.2551	2.3954	0.062215
28	0.8638	1.0067	1.0159	0.0091388	2.2808	2.4239	0.062741
29	0.8713	1.0067	1.0142	0.0074501	2.2856	2.4515	0.072585
30	0.8801	1.0063	1.0123	0.0059624	2.2957	2.4844	0.082197
31	0.8911	1.0057	1.0101	0.0043751	2.3121	2.5264	0.092686
32	0.9031	1.0051	1.0079	0.0027858	2.3094	2.5735	0.114359
33	0.9136	1.0039	1.0063	0.0023907	2.3544	2.6157	0.110984
34	0.9263	1.0035	1.0046	0.0010962	2.3644	2.6680	0.128405
35	0.9344	1.0014	1.0036	0.0021969	2.4221	2.7022	0.115643
36	0.9480	1.0011	1.0023	0.0011987	2.4432	2.7610	0.130075
37	0.9528	1.0001	1.0019	0.0017998	2.4777	2.7822	0.122896
Sum of data		53.3372	54.8178	0.8348223	64.0876	67.3229	1.497707

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1exp}}{\gamma_{1exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2exp}}{\gamma_{2exp}}\right)\right|\right] x100$$

= ((0.8348223+1.497707) x 100)/37

= 6.30%

Table5.12 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = 1.15A_{21}.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert (\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp} \rvert$	γ_{2exp}	γ_{2exp}	$\lvert (\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp} \rvert$
1	0.0874	3.4513	3.0846	0.1062498	1.0187	1.0239	0.005105
2	0.0967	3.3591	2.9503	0.1216993	1.0192	1.0285	0.009125
3	0.1411	2.8214	2.4503	0.1315304	1.0463	1.0545	0.007837
4	0.1756	2.4675	2.1743	0.1188247	1.0731	1.0784	0.004939
5	0.2065	2.2331	1.9820	0.1124446	1.0995	1.1022	0.002456
6	0.2253	2.0935	1.8840	0.1000717	1.1181	1.1177	0.000358
7	0.2252	1.9235	1.8845	0.0202755	1.1505	1.1176	0.028596
8	0.2856	1.7856	1.6395	0.0818212	1.1822	1.1720	0.008628
9	0.3133	1.6845	1.5537	0.0776492	1.2124	1.1993	0.010805
10	0.3535	1.5497	1.4503	0.0641414	1.2689	1.2412	0.02183
11	0.3773	1.4861	1.3986	0.0588789	1.2967	1.2674	0.022596
12	0.3999	1.4325	1.3550	0.0541012	1.3258	1.2932	0.024589
13	0.4258	1.3738	1.311	0.0457126	1.3637	1.3238	0.029259
14	0.4691	1.2973	1.2477	0.0382333	1.4273	1.3776	0.034821
15	0.4987	1.2495	1.2113	0.0305722	1.4825	1.4163	0.044654
16	0.5218	1.2158	1.1862	0.0243461	1.5257	1.4476	0.05119
17	0.5421	1.1950	1.1661	0.0241841	1.5551	1.4759	0.050929
18	0.5692	1.1688	1.1420	0.0229295	1.5971	1.5149	0.051468
19	0.5907	1.1436	1.1249	0.0163519	1.6439	1.5469	0.059006
20	0.6242	1.1148	1.1013	0.0121098	1.7106	1.5984	0.065591
21	0.6697	1.0817	1.0746	0.0065637	1.8037	1.6720	0.073017
22	0.6868	1.0716	1.0659	0.0053191	1.8439	1.7007	0.077661
23	0.7586	1.0366	1.0367	0.0000965	2.0159	1.8284	0.093011
24	0.7811	1.0266	1.0296	0.0029223	2.0754	1.8708	0.098583

Table5.12 (continued).

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert (\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp} \rvert$	γ_{2exp}	γ_{2exp}	$\lvert (\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp} \rvert$
25	0.8299	1.0129	1.0172	0.0042452	2.1990	1.9669	0.105548
26	0.8454	1.0119	1.0140	0.0020753	2.2319	1.9986	0.104530
27	0.8559	1.0090	1.0121	0.0030723	2.2551	2.0205	0.104031
28	0.8638	1.0067	1.0107	0.0039734	2.2808	2.0371	0.106848
29	0.8713	1.0067	1.0095	0.0027814	2.2856	2.0530	0.101768
30	0.8801	1.0063	1.0082	0.0018881	2.2957	2.0719	0.097487
31	0.8911	1.0057	1.0067	0.0009943	2.3121	2.0958	0.093551
32	0.9031	1.0051	1.0053	0.0001990	2.3094	2.1222	0.081060
33	0.9136	1.0039	1.0042	0.0002988	2.3544	2.1456	0.088685
34	0.9263	1.0035	1.003	0.0004983	2.3644	2.1744	0.080359
35	0.9344	1.0014	1.0024	0.0009986	2.4221	2.1930	0.094587
36	0.9480	1.0011	1.0015	0.0003996	2.4432	2.2246	0.089473
37	0.9528	1.0001	1.0012	0.0010999	2.4777	2.2359	0.097591
Sum of data		53.3372	50.6004	1.2995533	64.0876	59.8087	2.12157

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1exp}}{\gamma_{1exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2exp}}{\gamma_{2exp}}\right)\right|\right]x100$$

$$= ((1.2995533+2.12157) \times 100)/37$$

$$= 9.25\%$$

Table5.13 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = $0.85A_{21}$.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\vert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\vert$	γ_{2exp}	γ_{2exp}	$\vert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\vert$
1	0.0874	3.4513	3.8180	0.1062498	1.0187	1.0256	0.006773
2	0.0967	3.3591	3.6386	0.0832068	1.0192	1.0306	0.011185
3	0.1411	2.8214	2.9706	0.0528815	1.0463	1.0590	0.012138
4	0.1756	2.4675	2.6021	0.0545491	1.0731	1.0857	0.011742
5	0.2065	2.2331	2.3452	0.0501993	1.0995	1.1126	0.011915
6	0.2253	2.0935	2.2143	0.0577024	1.1181	1.1304	0.011001
7	0.2252	1.9235	2.2149	0.1514947	1.1505	1.1303	0.01756
8	0.2856	1.7856	1.8867	0.0566196	1.1822	1.1940	0.009981
9	0.3133	1.6845	1.7713	0.0515286	1.2124	1.2266	0.011712
10	0.3535	1.5497	1.6319	0.0530425	1.2689	1.2779	0.007093
11	0.3773	1.4861	1.5620	0.0510733	1.2967	1.3100	0.010257
12	0.3999	1.4325	1.5027	0.0490052	1.3258	1.3431	0.013049
13	0.4258	1.3738	1.4422	0.0497889	1.3637	1.3824	0.013713
14	0.4691	1.2973	1.3559	0.0451707	1.4273	1.4533	0.018216
15	0.4987	1.2495	1.3057	0.0449780	1.4825	1.5055	0.015514
16	0.5218	1.2158	1.2708	0.0452377	1.5257	1.5487	0.015075
17	0.5421	1.1950	1.2428	0.0400000	1.5551	1.5883	0.021349
18	0.5692	1.1688	1.2090	0.0343943	1.5971	1.6440	0.029366
19	0.5907	1.1436	1.1848	0.0360266	1.6439	1.6905	0.028347
20	0.6242	1.1148	1.1513	0.0327413	1.7106	1.7673	0.033146
21	0.6697	1.0817	1.1128	0.0287510	1.8037	1.8810	0.042856
22	0.6868	1.0716	1.1002	0.0266891	1.8439	1.9267	0.044905
23	0.7586	1.0366	1.0569	0.0195833	2.0159	2.1386	0.060866
24	0.7811	1.0266	1.0463	0.0191896	2.0754	2.2124	0.066011

Table5.13 (continued).

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
25	0.8299	1.0129	1.0273	0.0142166	2.1990	2.3862	0.085130
26	0.8454	1.0119	1.0224	0.0103765	2.2319	2.4457	0.095793
27	0.8559	1.0090	1.0194	0.0103072	2.2551	2.4872	0.102922
28	0.8638	1.0067	1.0173	0.0105295	2.2808	2.5192	0.104525
29	0.8713	1.0067	1.0154	0.0086421	2.2856	2.5501	0.115725
30	0.8801	1.0063	1.0133	0.0069562	2.2957	2.5871	0.126933
31	0.8911	1.0057	1.0110	0.0052700	2.3121	2.6344	0.139397
32	0.9031	1.0051	1.0086	0.0034822	2.3094	2.6875	0.163722
33	0.9136	1.0039	1.0069	0.0029883	2.3544	2.7353	0.161782
34	0.9263	1.0035	1.0050	0.0014948	2.3644	2.7947	0.181991
35	0.9344	1.0014	1.0039	0.0024965	2.4221	2.8337	0.169935
36	0.9480	1.0011	1.0025	0.0013985	2.4432	2.9008	0.187295
37	0.9528	1.0001	1.0020	0.0018998	2.4777	2.9250	0.180530
Sum of data		53.3372	55.792	1.3201615	64.0876	69.1514	2.339449

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1exp}}{\gamma_{1exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2exp}}{\gamma_{2exp}}\right)\right|\right]\text{x}100$$

= ((1.3201615+2.339449) x 100)/37

= 9.99%

Table5.14 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = 1.20A_{21}.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
1	0.0874	3.4513	2.9796	0.1366731	1.0187	1.0236	0.00481
2	0.0967	3.3591	2.8518	0.1510226	1.0192	1.0281	0.008732
3	0.1411	2.8214	2.3760	0.1578649	1.0463	1.0536	0.006977
4	0.1756	2.4675	2.1134	0.1435056	1.0731	1.0770	0.003672
5	0.2065	2.2331	1.9304	0.1355515	1.0995	1.1003	0.000728
6	0.2253	2.0935	1.8372	0.1224266	1.1181	1.1154	0.002415
7	0.2252	1.9235	1.8377	0.0446062	1.1505	1.1153	0.030595
8	0.2856	1.7856	1.6047	0.1013105	1.1822	1.1681	0.011927
9	0.3133	1.6845	1.5231	0.0958148	1.2124	1.1945	0.014764
10	0.3535	1.5497	1.4249	0.0805317	1.2689	1.2349	0.026795
11	0.3773	1.4861	1.3759	0.0741538	1.2967	1.2600	0.028303
12	0.3999	1.4325	1.3345	0.0684119	1.3258	1.2847	0.031000
13	0.4258	1.3738	1.2925	0.0591789	1.3637	1.3140	0.036445
14	0.4691	1.2973	1.2328	0.0497186	1.4273	1.3651	0.043537
15	0.4987	1.2495	1.1984	0.0408964	1.4825	1.4018	0.054435
16	0.5218	1.2158	1.1747	0.0338049	1.5257	1.4314	0.061808
17	0.5421	1.1950	1.1557	0.0328870	1.5551	1.4581	0.062375
18	0.5692	1.1688	1.1330	0.0306297	1.5971	1.4947	0.064116
19	0.5907	1.1436	1.1169	0.0233473	1.6439	1.5246	0.072571
20	0.6242	1.1148	1.0947	0.0180301	1.7106	1.5726	0.080673
21	0.6697	1.0817	1.0696	0.0111861	1.8037	1.6409	0.090259
22	0.6868	1.0716	1.0614	0.0095185	1.8439	1.6675	0.095667
23	0.7586	1.0366	1.0340	0.0025082	2.0159	1.7848	0.114639
24	0.7811	1.0266	1.0274	0.0007793	2.0754	1.8234	0.121422

Table5.14 (continued).

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert (\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp} \rvert$	γ_{2exp}	γ_{2exp}	$\lvert (\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp} \rvert$
25	0.8299	1.0129	1.0159	0.0029618	2.1990	1.9106	0.131151
26	0.8454	1.0119	1.0130	0.0010871	2.2319	1.9393	0.131099
27	0.8559	1.0090	1.0112	0.0021804	2.2551	1.9589	0.131347
28	0.8638	1.0067	1.0099	0.0031787	2.2808	1.9739	0.134558
29	0.8713	1.0067	1.0088	0.0020860	2.2856	1.9882	0.130119
30	0.8801	1.0063	1.0076	0.0012919	2.2957	2.0052	0.126541
31	0.8911	1.0057	1.0062	0.0004972	2.3121	2.0266	0.123481
32	0.9031	1.0051	1.0049	0.0001990	2.3094	2.0502	0.112237
33	0.9136	1.0039	1.0039	0.0000000	2.3544	2.0711	0.120328
34	0.9263	1.0035	1.0028	0.0006976	2.3644	2.0967	0.113221
35	0.9344	1.0014	1.0022	0.0007989	2.4221	2.1133	0.127493
36	0.9480	1.0011	1.0014	0.0002997	2.4432	2.1413	0.123567
37	0.9528	1.0001	1.0011	0.0009999	2.4777	2.1513	0.131735
Sum of data		53.3372	49.8692	1.6406361	64.0876	58.5611	2.705541

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1exp}}{\gamma_{1exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2exp}}{\gamma_{2exp}}\right)\right|\right]x100$$

= ((1.6406361+2.705541) x 100)/37

= 11.75%

Table5.15 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = 0.80A_{21}.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert (\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp} \rvert$	γ_{2exp}	γ_{2exp}	$\lvert (\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp} \rvert$
1	0.0874	3.4513	3.9599	0.1473648	1.0187	1.0258	0.006970
2	0.0967	3.3591	3.7718	0.1228603	1.0192	1.0309	0.011480
3	0.1411	2.8214	3.0718	0.0887503	1.0463	1.0597	0.012807
4	0.1756	2.4675	2.6855	0.0883485	1.0731	1.0867	0.012674
5	0.2065	2.2331	2.4163	0.0820384	1.0995	1.1142	0.013370
6	0.2253	2.0935	2.2790	0.0886076	1.1181	1.1322	0.012611
7	0.2252	1.9235	2.2797	0.1851833	1.1505	1.1321	0.015993
8	0.2856	1.7856	1.9355	0.0839494	1.1822	1.1973	0.012773
9	0.3133	1.6845	1.8144	0.0771149	1.2124	1.2308	0.015177
10	0.3535	1.5497	1.6681	0.0764019	1.2689	1.2836	0.011585
11	0.3773	1.4861	1.5947	0.0730772	1.2967	1.3173	0.015886
12	0.3999	1.4325	1.5324	0.0697382	1.3258	1.3511	0.019083
13	0.4258	1.3738	1.4688	0.0691513	1.3637	1.3919	0.020679
14	0.4691	1.2973	1.3779	0.0621290	1.4273	1.4658	0.026974
15	0.4987	1.2495	1.3250	0.0604242	1.4825	1.5201	0.025363
16	0.5218	1.2158	1.2882	0.0595493	1.5257	1.5659	0.026349
17	0.5421	1.1950	1.2586	0.0532218	1.5551	1.6077	0.033824
18	0.5692	1.1688	1.2229	0.0462868	1.5971	1.6666	0.043516
19	0.5907	1.1436	1.1973	0.0469570	1.6439	1.716	0.043859
20	0.6242	1.1148	1.1618	0.0421600	1.7106	1.7979	0.051035
21	0.6697	1.0817	1.1209	0.0362393	1.8037	1.9198	0.064368
22	0.6868	1.0716	1.1075	0.0335013	1.8439	1.9691	0.067900
23	0.7586	1.0366	1.0614	0.0239244	2.0159	2.1998	0.091225
24	0.7811	1.0266	1.0499	0.0226963	2.0754	2.2809	0.099017

Table5.15 (continued).

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
25	0.8299	1.0129	1.0296	0.0164873	2.1990	2.4733	0.124739
26	0.8454	1.0119	1.0243	0.0122542	2.2319	2.5397	0.137909
27	0.8559	1.0090	1.0211	0.0119921	2.2551	2.5862	0.146823
28	0.8638	1.0067	1.0188	0.0120195	2.2808	2.6220	0.149597
29	0.8713	1.0067	1.0167	0.0099334	2.2856	2.6568	0.162408
30	0.8801	1.0063	1.0145	0.0081487	2.2957	2.6984	0.175415
31	0.8911	1.0057	1.0119	0.0061649	2.3121	2.7519	0.190217
32	0.9031	1.0051	1.0094	0.0042782	2.3094	2.8120	0.217632
33	0.9136	1.0039	1.0075	0.0035860	2.3544	2.8663	0.217423
34	0.9263	1.0035	1.0054	0.0018934	2.3644	2.9340	0.240907
35	0.9344	1.0014	1.0043	0.0028959	2.4221	2.9785	0.229718
36	0.9480	1.0011	1.0027	0.0015982	2.4432	3.0554	0.250573
37	0.9528	1.0001	1.0022	0.0020998	2.4777	3.0833	0.24442
Sum of data		53.3372	56.8177	1.8330267	64.0876	71.121	3.242294

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1exp}}{\gamma_{1exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2exp}}{\gamma_{2exp}}\right)\right|\right]x100$$

= ((1.8330267+3.242294) x 100)/37

= 13.72%

Table5.16 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = 1.25A_{21}.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
1	0.0874	3.4513	2.8788	0.1658795	1.0187	1.0232	0.004417
2	0.0967	3.3591	2.7573	0.1791551	1.0192	1.0277	0.008340
3	0.1411	2.8214	2.3048	0.1831006	1.0463	1.0527	0.006117
4	0.1756	2.4675	2.0550	0.1671733	1.0731	1.0757	0.002423
5	0.2065	2.2331	1.8810	0.1576732	1.0995	1.0983	0.001090
6	0.2253	2.0935	1.7924	0.1438261	1.1181	1.1130	0.004561
7	0.2252	1.9235	1.7929	0.0678971	1.1505	1.1129	0.032681
8	0.2856	1.7856	1.5714	0.1199597	1.1822	1.1642	0.015226
9	0.3133	1.6845	1.4939	0.1131493	1.2124	1.1896	0.018806
10	0.3535	1.5497	1.4007	0.0961476	1.2689	1.2285	0.031839
11	0.3773	1.4861	1.3542	0.0887558	1.2967	1.2526	0.034009
12	0.3999	1.4325	1.3150	0.0820244	1.3258	1.2762	0.037411
13	0.4258	1.3738	1.2752	0.0717717	1.3637	1.3041	0.043705
14	0.4691	1.2973	1.2187	0.0605874	1.4273	1.3528	0.052196
15	0.4987	1.2495	1.1862	0.0506603	1.4825	1.3875	0.064081
16	0.5218	1.2158	1.1638	0.0427702	1.5257	1.4153	0.072360
17	0.5421	1.1950	1.1459	0.0410879	1.5551	1.4404	0.073757
18	0.5692	1.1688	1.1245	0.0379021	1.5971	1.4748	0.076576
19	0.5907	1.1436	1.1093	0.029993	1.6439	1.5028	0.085832
20	0.6242	1.1148	1.0884	0.0236814	1.7106	1.5476	0.095288
21	0.6697	1.0817	1.0648	0.0156236	1.8037	1.6109	0.106891
22	0.6868	1.0716	1.0572	0.0134378	1.8439	1.6354	0.113076
23	0.7586	1.0366	1.0316	0.0048235	2.0159	1.74304	0.135354
24	0.7811	1.0266	1.0254	0.0011689	2.0754	1.7783	0.143153

Table5.16 (continued)

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
25	0.8299	1.0129	1.0147	0.0017771	2.1990	1.8574	0.155343
26	0.8454	1.0119	1.0120	0.0000988	2.2319	1.8833	0.156190
27	0.8559	1.0090	1.0103	0.0012884	2.2551	1.9010	0.157022
28	0.8638	1.0067	1.0092	0.0024834	2.2808	1.9145	0.160602
29	0.8713	1.0067	1.0081	0.0013907	2.2856	1.9273	0.156764
30	0.8801	1.0063	1.0070	0.0006956	2.2957	1.9425	0.153853
31	0.8911	1.0057	1.0057	0.0000000	2.3121	1.9617	0.151551
32	0.9031	1.0051	1.0045	0.0005970	2.3094	1.9829	0.141379
33	0.9136	1.0039	1.0035	0.0003984	2.3544	2.0016	0.149847
34	0.9263	1.0035	1.0026	0.0008969	2.3644	2.0244	0.143810
35	0.9344	1.0014	1.0020	0.0005992	2.4221	2.0391	0.158127
36	0.9480	1.0011	1.0012	0.0000999	2.4432	2.0641	0.155165
37	0.9528	1.0001	1.0010	0.0008999	2.4777	2.0730	0.163337
Sum of data		53.3372	49.1702	1.9694746	64.0876	57.3803	3.262172

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1exp}}{\gamma_{1exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2exp}}{\gamma_{2exp}}\right)\right|\right]x100$$

= ((1.9694746+3.262172) x 100)/37

= 14.14%

Table5.17 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = 0.75A_{21}.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
1	0.0874	3.4513	4.1081	0.1903051	1.0187	1.0260	0.007166
2	0.0967	3.3591	3.9111	0.1643297	1.0192	1.0311	0.011676
3	0.1411	2.8214	3.1776	0.1262494	1.0463	1.0603	0.013380
4	0.1756	2.4675	2.7730	0.1238095	1.0731	1.0878	0.013699
5	0.2065	2.2331	2.4909	0.1154449	1.0995	1.1156	0.014643
6	0.2253	2.0935	2.3470	0.1210891	1.1181	1.1340	0.014221
7	0.2252	1.9235	2.3478	0.2205875	1.1505	1.1339	0.014429
8	0.2856	1.7856	1.9870	0.1127912	1.1822	1.2005	0.015480
9	0.3133	1.6845	1.8600	0.1041852	1.2124	1.2349	0.018558
10	0.3535	1.5497	1.7064	0.1011163	1.2689	1.2892	0.015998
11	0.3773	1.4861	1.6293	0.0963596	1.2967	1.3240	0.021053
12	0.3999	1.4325	1.5639	0.0917277	1.3258	1.3589	0.024966
13	0.4258	1.3738	1.497	0.0896783	1.3637	1.4013	0.027572
14	0.4691	1.2973	1.4013	0.0801665	1.4273	1.4782	0.035662
15	0.4987	1.2495	1.3456	0.0769108	1.4825	1.5355	0.035750
16	0.5218	1.2158	1.3067	0.0747656	1.5257	1.5831	0.037622
17	0.5421	1.1950	1.2756	0.0674477	1.5551	1.6272	0.046364
18	0.5692	1.1688	1.2379	0.0591205	1.5971	1.6894	0.057792
19	0.5907	1.1436	1.2108	0.0587618	1.6439	1.7417	0.059493
20	0.6242	1.1148	1.1731	0.0522964	1.7106	1.8290	0.069215
21	0.6697	1.0817	1.1297	0.0443746	1.8037	1.9598	0.086544
22	0.6868	1.0716	1.1154	0.0408735	1.8439	2.0130	0.091708
23	0.7586	1.0366	1.0662	0.0285549	2.0159	2.2642	0.123171
24	0.7811	1.0266	1.0540	0.0266900	2.0754	2.3533	0.133902

Table5.17 (continued)

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert (\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp} \rvert$	γ_{2exp}	γ_{2exp}	$\lvert (\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp} \rvert$
25	0.8299	1.0129	1.0321	0.0189555	2.1990	2.5667	0.167212
26	0.8454	1.0119	1.0264	0.0143295	2.2319	2.6409	0.183252
27	0.8559	1.0090	1.0229	0.0137760	2.2551	2.6931	0.194226
28	0.8638	1.0067	1.0204	0.0136088	2.2808	2.7334	0.198439
29	0.8713	1.0067	1.0182	0.0114235	2.2856	2.7725	0.213029
30	0.8801	1.0063	1.0158	0.0094405	2.2957	2.8195	0.228166
31	0.8911	1.0057	1.0130	0.0072586	2.3121	2.8800	0.245621
32	0.9031	1.0051	1.0100	0.0048751	2.3094	2.9484	0.276695
33	0.9136	1.0039	1.0082	0.0042833	2.3544	3.0103	0.278585
34	0.9263	1.0035	1.0059	0.0023916	2.3644	3.0878	0.305955
35	0.9344	1.0014	1.0047	0.0032954	2.4221	3.1388	0.295900
36	0.9480	1.0011	1.0029	0.0017980	2.4432	3.2275	0.321013
37	0.9528	1.0001	1.0024	0.0022998	2.4777	3.2597	0.315615
Sum of data		53.3372	57.8983	2.3753714	64.0876	73.2505	4.213773

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1\exp}}{\gamma_{1\exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2\exp}}{\gamma_{2\exp}}\right)\right|\right]\text{x100}$$

= ((2.3753714+4.213773) x 100)/37

= 17.81%

Table5.18 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = 1.30A_{21}.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
1	0.0874	3.4513	2.7821	0.1938980	1.0187	1.0229	0.004123
2	0.0967	3.3591	2.6667	0.2061266	1.0192	1.0273	0.007947
3	0.1411	2.8214	2.2365	0.2073084	1.0463	1.0518	0.005257
4	0.1756	2.4675	1.9991	0.1898278	1.0731	1.0742	0.001025
5	0.2065	2.2331	1.8337	0.1788545	1.0995	1.0963	0.002910
6	0.2253	2.0935	1.7495	0.1643181	1.1181	1.1106	0.006708
7	0.2252	1.9235	1.7499	0.0902521	1.1505	1.1105	0.034767
8	0.2856	1.7856	1.5390	0.1381048	1.1822	1.1602	0.018609
9	0.3133	1.6845	1.466	0.1297121	1.2124	1.1847	0.022847
10	0.3535	1.5497	1.3776	0.1110538	1.2689	1.2221	0.036882
11	0.3773	1.4861	1.3335	0.1026849	1.2967	1.2451	0.039793
12	0.3999	1.4325	1.2964	0.0950087	1.3258	1.2677	0.043823
13	0.4258	1.3738	1.2587	0.0837822	1.3637	1.2943	0.050891
14	0.4691	1.2973	1.2053	0.0709165	1.4273	1.3405	0.060814
15	0.4987	1.2495	1.1746	0.0599440	1.4825	1.3733	0.073659
16	0.5218	1.2158	1.1534	0.0513242	1.5257	1.3995	0.082716
17	0.5421	1.1950	1.1366	0.0488703	1.5551	1.4231	0.084882
18	0.5692	1.1688	1.1164	0.0448323	1.5971	1.4553	0.088786
19	0.5907	1.1436	1.1021	0.0362889	1.6439	1.4814	0.098850
20	0.6242	1.1148	1.0825	0.0289738	1.7106	1.5231	0.109611
21	0.6697	1.0817	1.0604	0.0196912	1.8037	1.5818	0.123025
22	0.6868	1.0716	1.0532	0.0171706	1.8439	1.6045	0.129834
23	0.7586	1.0366	1.0293	0.0070423	2.0159	1.7031	0.155166
24	0.7811	1.0266	1.0236	0.0029223	2.0754	1.7353	0.163872

Table5.18 (continued)

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
25	0.8299	1.0129	1.0136	0.0006911	2.1990	1.8070	0.178263
26	0.8454	1.0119	1.0111	0.0007906	2.2319	1.8303	0.179936
27	0.8559	1.0090	1.0095	0.0004955	2.2551	1.8463	0.181278
28	0.8638	1.0067	1.0085	0.0017880	2.2808	1.8584	0.185198
29	0.8713	1.0067	1.0075	0.0007947	2.2856	1.8700	0.181834
30	0.8801	1.0063	1.0065	0.0001987	2.2957	1.8837	0.179466
31	0.8911	1.0057	1.0053	0.0003977	2.3121	1.9009	0.177847
32	0.9031	1.0051	1.0041	0.0009949	2.3094	1.9198	0.168702
33	0.9136	1.0039	1.0033	0.0005977	2.3544	1.9365	0.177497
34	0.9263	1.0035	1.0024	0.0010962	2.3644	1.9569	0.172348
35	0.9344	1.0014	1.0019	0.0004993	2.4221	1.9700	0.186656
36	0.9480	1.0011	1.0012	0.0000999	2.4432	1.9922	0.184594
37	0.9528	1.0001	1.0009	0.0007999	2.4777	2.0001	0.192759
Sum of data		53.3372	48.5019	2.2881527	64.0876	56.2607	3.793178

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1exp}}{\gamma_{1exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2exp}}{\gamma_{2exp}}\right)\right|\right]\text{x}100$$

= ((2.2881527+3.793178) x 100)/37

= 16.44%

Table5.19 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = 0.70A_{21}.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
1	0.0874	3.4513	4.2631	0.2352157	1.0187	1.0262	0.007362
2	0.0967	3.3591	4.0567	0.2076747	1.0192	1.0314	0.011970
3	0.1411	2.8214	3.2885	0.1655561	1.0463	1.0610	0.014050
4	0.1756	2.4675	2.8647	0.1609726	1.0731	1.0887	0.014537
5	0.2065	2.2331	2.5693	0.1505530	1.0995	1.1170	0.015916
6	0.2253	2.0935	2.4185	0.1552424	1.1181	1.1358	0.015830
7	0.2252	1.9235	2.4193	0.2577593	1.1505	1.1357	0.012864
8	0.2856	1.7856	2.0412	0.1431452	1.1822	1.2035	0.018017
9	0.3133	1.6845	1.9080	0.1326803	1.2124	1.2388	0.021775
10	0.3535	1.5497	1.7469	0.1272504	1.2689	1.2947	0.020333
11	0.3773	1.4861	1.6659	0.1209878	1.2967	1.3305	0.026066
12	0.3999	1.4325	1.5972	0.1149738	1.3258	1.3666	0.030774
13	0.4258	1.3738	1.527	0.1115155	1.3637	1.4105	0.034318
14	0.4691	1.2973	1.4263	0.0994373	1.4273	1.4905	0.044279
15	0.4987	1.2495	1.3676	0.0945178	1.4825	1.5504	0.045801
16	0.5218	1.2158	1.3267	0.0912157	1.5257	1.6003	0.048896
17	0.5421	1.195	1.2938	0.0826778	1.5551	1.6466	0.058839
18	0.5692	1.1688	1.2539	0.0728097	1.5971	1.7123	0.072131
19	0.5907	1.1436	1.2253	0.0714411	1.6439	1.7678	0.075370
20	0.6242	1.1148	1.1854	0.0633297	1.7106	1.8607	0.087747
21	0.6697	1.0817	1.1393	0.0532495	1.8037	2.001	0.109386
22	0.6868	1.0716	1.1241	0.0489922	1.8439	2.0584	0.11633
23	0.7586	1.0366	1.0715	0.0336678	2.0159	2.3319	0.156754
24	0.7811	1.0266	1.0584	0.0309760	2.0754	2.4300	0.170859

Table5.19 (continued)

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
25	0.8299	1.0129	1.0349	0.0217198	2.1990	2.6670	0.212824
26	0.8454	1.0119	1.0287	0.0166024	2.2319	2.7501	0.232179
27	0.8559	1.0090	1.0249	0.0157582	2.2551	2.8088	0.245532
28	0.8638	1.0067	1.0222	0.0153968	2.2808	2.8542	0.251403
29	0.8713	1.0067	1.0198	0.0130128	2.2856	2.8984	0.268113
30	0.8801	1.0063	1.0172	0.0108318	2.2957	2.9517	0.285752
31	0.8911	1.0057	1.0142	0.0084518	2.3121	3.0205	0.306388
32	0.9031	1.0051	1.0112	0.0060690	2.3094	3.0985	0.341690
33	0.9136	1.0039	1.0089	0.0049806	2.3544	3.1693	0.346118
34	0.9263	1.0035	1.0065	0.0029895	2.3644	3.2584	0.378109
35	0.9344	1.0014	1.0052	0.0037947	2.4221	3.3173	0.369597
36	0.9480	1.0011	1.0032	0.0020977	2.4432	3.4199	0.399763
37	0.9528	1.0001	1.0027	0.0025997	2.4777	3.4573	0.395367
Sum of data		53.3372	59.0382	2.9501465	64.0876	75.5617	5.263038

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1exp}}{\gamma_{1exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2exp}}{\gamma_{2exp}}\right)\right|\right]\text{x}100$$

= ((2.9504165+5.263038) x 100)/37

= 22.20%

Table5.20 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = 1.35A_{21}.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
1	0.0874	3.4513	2.6894	0.2207574	1.0187	1.0226	0.003828
2	0.0967	3.3591	2.5797	0.2320264	1.0192	1.0269	0.007555
3	0.1411	2.8214	2.171	0.2305239	1.0463	1.0509	0.004396
4	0.1756	2.4675	1.9454	0.2115907	1.0731	1.0728	0.000280
5	0.2065	2.2331	1.7883	0.1991850	1.0995	1.0943	0.004729
6	0.2253	2.0935	1.7084	0.1839503	1.1181	1.10815	0.008899
7	0.2252	1.9235	1.7088	0.1116194	1.1505	1.1081	0.036854
8	0.2856	1.7856	1.5091	0.1548499	1.1822	1.1561	0.022077
9	0.3133	1.6845	1.4393	0.1455625	1.2124	1.1797	0.026971
10	0.3535	1.5497	1.3555	0.1253146	1.2689	1.2156	0.042005
11	0.3773	1.4861	1.3138	0.1159411	1.2967	1.2377	0.045500
12	0.3999	1.4325	1.2786	0.1074346	1.3258	1.2592	0.050234
13	0.4258	1.3738	1.2429	0.0952832	1.3637	1.2845	0.058077
14	0.4691	1.2973	1.1925	0.0807832	1.4273	1.3283	0.069362
15	0.4987	1.2495	1.1635	0.0688275	1.4825	1.3592	0.083170
16	0.5218	1.2158	1.1435	0.0594670	1.5257	1.3839	0.092941
17	0.5421	1.1950	1.1277	0.056318	1.5551	1.4061	0.095814
18	0.5692	1.1688	1.1087	0.0514203	1.5971	1.4362	0.100745
19	0.5907	1.1436	1.0953	0.042235	1.6439	1.4606	0.111503
20	0.6242	1.1148	1.0769	0.0339971	1.7106	1.4994	0.123465
21	0.6697	1.0817	1.0562	0.0235740	1.8037	1.5536	0.138659
22	0.6868	1.0716	1.0495	0.0206234	1.8439	1.5745	0.146103
23	0.7586	1.0366	1.0272	0.0090681	2.0159	1.6650	0.174066
24	0.7811	1.0266	1.0218	0.0046756	2.0754	1.6942	0.183675

Table5.20 (continued)

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
25	0.8299	1.0129	1.0126	0.0002962	2.1990	1.7592	0.200000
26	0.8454	1.0119	1.0102	0.0016800	2.2319	1.7803	0.202339
27	0.8559	1.009	1.0088	0.0001982	2.2551	1.7947	0.204159
28	0.8638	1.0067	1.0078	0.0010927	2.2808	1.8056	0.208348
29	0.8713	1.0067	1.0069	0.0001987	2.2856	1.8160	0.205460
30	0.8801	1.0063	1.0060	0.0002981	2.2957	1.8283	0.203598
31	0.8911	1.0057	1.0049	0.0007955	2.3121	1.8437	0.202586
32	0.9031	1.0051	1.0038	0.0012934	2.3094	1.8606	0.194336
33	0.9136	1.0039	1.0030	0.0008965	2.3544	1.8756	0.203364
34	0.9263	1.0035	1.0022	0.0012955	2.3644	1.8938	0.199036
35	0.9344	1.0014	1.0020	0.0005992	2.4221	1.9054	0.213327
36	0.9480	1.0011	1.0010	0.0000999	2.4432	1.9252	0.212017
37	0.9528	1.0001	1.0010	0.0008999	2.4777	1.9322	0.220164
Sum of data		53.3372	47.8632	2.5946718	64.0876	55.1981	4.299646

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1exp}}{\gamma_{1exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2exp}}{\gamma_{2exp}}\right)\right|\right]\text{x100}$$

$$= ((2.5946718+4.299646) \text{ x } 100)/37$$

$$= 18.63\%$$

Table5.21 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = 0.65A_{21}.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
1	0.0874	3.4513	4.4252	0.2821835	1.0187	1.0264	0.007559
2	0.0967	3.3591	4.209	0.2530142	1.0192	1.0316	0.012166
3	0.1411	2.8214	3.4048	0.2067768	1.0463	1.0614	0.014432
4	0.1756	2.4675	2.9610	0.2000000	1.0731	1.0896	0.015376
5	0.2065	2.2331	2.6517	0.1874524	1.0995	1.1184	0.017190
6	0.2253	2.0935	2.4938	0.1912109	1.1181	1.1374	0.017261
7	0.2252	1.9235	2.4946	0.2969067	1.1505	1.1373	0.011473
8	0.2856	1.7856	2.0985	0.1752352	1.1822	1.2066	0.020639
9	0.3133	1.6845	1.9589	0.1628970	1.2124	1.2426	0.024909
10	0.3535	1.5497	1.7899	0.1549977	1.2689	1.2999	0.024431
11	0.3773	1.4861	1.7049	0.147231	1.2967	1.3368	0.030925
12	0.3999	1.4325	1.6328	0.1398255	1.3258	1.3741	0.036431
13	0.4258	1.3738	1.5589	0.1347358	1.3637	1.4195	0.040918
14	0.4691	1.2973	1.4530	0.1200185	1.4273	1.5026	0.052757
15	0.4987	1.2495	1.3912	0.1134054	1.4825	1.5651	0.055717
16	0.5218	1.2158	1.3480	0.1087350	1.5257	1.6174	0.060104
17	0.5421	1.1950	1.3133	0.0989958	1.5551	1.6661	0.071378
18	0.5692	1.1688	1.2712	0.0876112	1.5971	1.7354	0.086594
19	0.5907	1.1436	1.2409	0.0850822	1.6439	1.7941	0.091368
20	0.6242	1.1148	1.1986	0.0751704	1.7106	1.8930	0.106629
21	0.6697	1.0817	1.1497	0.0628640	1.8037	2.0433	0.132838
22	0.6868	1.0716	1.1335	0.0577641	1.8439	2.1051	0.141656
23	0.7586	1.0366	1.0774	0.0393594	2.0159	2.4031	0.192073
24	0.7811	1.0266	1.0633	0.0357491	2.0754	2.5111	0.209935

Table5.21 (continued)

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
25	0.8299	1.0129	1.0380	0.0247803	2.1990	2.7749	0.261892
26	0.8454	1.0119	1.0313	0.0191719	2.2319	2.8683	0.285138
27	0.8559	1.0090	1.0272	0.0180377	2.2551	2.9344	0.301228
28	0.8638	1.0067	1.0243	0.0174829	2.2808	2.9858	0.309102
29	0.8713	1.0067	1.0217	0.0149002	2.2856	3.0360	0.328316
30	0.8801	1.0063	1.0199	0.0135149	2.2957	3.0965	0.348826
31	0.8911	1.0057	1.0155	0.0097445	2.3121	3.1750	0.373211
32	0.9031	1.0051	1.0123	0.0071635	2.3094	3.2644	0.413527
33	0.9136	1.0039	1.0098	0.0058771	2.3544	3.3458	0.421084
34	0.9263	1.0035	1.0071	0.0035874	2.3644	3.4488	0.458636
35	0.9344	1.0014	1.0057	0.0042940	2.4221	3.5171	0.452087
36	0.9480	1.0011	1.0036	0.0024973	2.4432	3.6367	0.488499
37	0.9528	1.0001	1.0029	0.0027997	2.4777	3.6804	0.485410
Sum of data		53.3372	60.2434	3.561073	64.0876	78.082	6.401717

N = number of data points

$$\%\text{Average Absolute Deviation} = \tfrac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1\exp}}{\gamma_{1\exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2\exp}}{\gamma_{2\exp}}\right)\right|\right]\text{x}100$$

= ((3.561073+6.401717) x 100)/37

= 26.93%

Table5.22 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = 1.40A_{21}.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
1	0.0874	3.4513	2.6003	0.2465738	1.0187	1.0222	0.003436
2	0.0967	3.3591	2.4962	0.2568843	1.0192	1.0265	0.007162
3	0.1411	2.8214	2.1081	0.2528178	1.0463	1.0500	0.003536
4	0.1756	2.4675	1.8939	0.2324620	1.0731	1.0713	0.001677
5	0.2065	2.2331	1.7448	0.2186646	1.0995	1.0922	0.006639
6	0.2253	2.0935	1.6689	0.2028182	1.1181	1.1057	0.011090
7	0.2252	1.9235	1.6693	0.1321549	1.1505	1.1056	0.039027
8	0.2856	1.7856	1.4799	0.1712030	1.1822	1.1520	0.025546
9	0.3133	1.6845	1.4137	0.1607599	1.2124	1.1747	0.031095
10	0.3535	1.5497	1.3343	0.1389946	1.2689	1.2091	0.047127
11	0.3773	1.4861	1.2948	0.1287262	1.2967	1.2302	0.051284
12	0.3999	1.4325	1.2616	0.1193019	1.3258	1.2507	0.056645
13	0.4258	1.3738	1.2279	0.1062018	1.3637	1.2747	0.065264
14	0.4691	1.2973	1.1803	0.0901873	1.4273	1.3162	0.077839
15	0.4987	1.2495	1.1530	0.0772309	1.4825	1.3453	0.092546
16	0.5218	1.2158	1.1342	0.0671163	1.5257	1.3686	0.102969
17	0.5421	1.1950	1.1192	0.0634310	1.5551	1.3893	0.106617
18	0.5692	1.1688	1.1014	0.0576660	1.5971	1.4175	0.112454
19	0.5907	1.1436	1.0888	0.0479189	1.6439	1.4402	0.123913
20	0.6242	1.1148	1.0716	0.0387513	1.7106	1.4762	0.137028
21	0.6697	1.0817	1.0522	0.0272719	1.8037	1.5264	0.153740
22	0.6868	1.0716	1.0459	0.0239828	1.8439	1.5456	0.161777
23	0.7586	1.0366	1.0251	0.011094	2.0159	1.6284	0.192222
24	0.7811	1.0266	1.0202	0.0062342	2.0754	1.6550	0.202563

Table5.22 (continued)

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
25	0.8299	1.0129	1.0116	0.0012834	2.1990	1.7139	0.220600
26	0.8454	1.0119	1.0094	0.0024706	2.2319	1.7329	0.223576
27	0.8559	1.0090	1.0081	0.0008920	2.2551	1.7458	0.225844
28	0.8638	1.0067	1.0072	0.0004967	2.2808	1.7556	0.230270
29	0.8713	1.0067	1.0064	0.0002980	2.2856	1.7650	0.227774
30	0.8801	1.0063	1.0055	0.0007950	2.2957	1.7760	0.226380
31	0.8911	1.0057	1.0045	0.0011932	2.3121	1.7898	0.225899
32	0.9031	1.0051	1.0035	0.0015919	2.3094	1.8049	0.218455
33	0.9136	1.0039	1.0028	0.0010957	2.3544	1.8183	0.227701
34	0.9263	1.0035	1.0020	0.0014948	2.3644	1.8345	0.224116
35	0.9344	1.0014	1.0016	0.0001997	2.4221	1.8449	0.238306
36	0.9480	1.0011	1.0010	0.0000999	2.4432	1.8625	0.237680
37	0.9528	1.0001	1.0008	0.0006999	2.4777	1.8687	0.245792
Sum of data		53.3372	47.25	2.8910583	64.0876	54.1864	4.78559

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1\exp}}{\gamma_{1\exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2\exp}}{\gamma_{2\exp}}\right)\right|\right]\text{x}100$$

$$= ((2.8910583+4.78559)\text{ x }100)/37$$

$$= 20.75\%$$

Table5.23 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = 0.60A_{21}.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
1	0.0874	3.4513	4.5947	0.3312955	1.0187	1.0266	0.007755
2	0.0967	3.3591	4.3685	0.3004972	1.0192	1.0319	0.012461
3	0.1411	2.8214	3.5267	0.2499823	1.0463	1.0620	0.015005
4	0.1756	2.4675	3.0622	0.2410132	1.0731	1.0905	0.016215
5	0.2065	2.2331	2.7383	0.2262326	1.0995	1.1196	0.018281
6	0.2253	2.0935	2.5730	0.2290423	1.1181	1.1390	0.018692
7	0.2252	1.9235	2.5739	0.3381336	1.1505	1.1390	0.009996
8	0.2856	1.7856	2.1590	0.2091174	1.1822	1.2094	0.023008
9	0.3133	1.6845	2.0168	0.1972692	1.2124	1.2462	0.027879
10	0.3535	1.5497	1.8355	0.1844228	1.2689	1.3050	0.028450
11	0.3773	1.4861	1.7463	0.1750892	1.2967	1.3429	0.035629
12	0.3999	1.4325	1.6706	0.1662129	1.3258	1.3813	0.041862
13	0.4258	1.3738	1.5930	0.1595574	1.3637	1.4283	0.047371
14	0.4691	1.2973	1.4816	0.1420643	1.4273	1.5145	0.061094
15	0.4987	1.2495	1.4166	0.1337335	1.4825	1.5797	0.065565
16	0.5218	1.2158	1.3710	0.1276526	1.5257	1.6344	0.071246
17	0.5421	1.1950	1.3344	0.1166527	1.5551	1.6854	0.083789
18	0.5692	1.1688	1.2899	0.1036105	1.5971	1.7584	0.100996
19	0.5907	1.1436	1.2579	0.0999475	1.6439	1.8206	0.107488
20	0.6242	1.1148	1.2131	0.0881773	1.7106	1.9256	0.125687
21	0.6697	1.0817	1.1611	0.0734030	1.8037	2.0866	0.156844
22	0.6868	1.0716	1.1439	0.0674692	1.8439	2.1533	0.167797
23	0.7586	1.0366	1.0839	0.0456299	2.0159	2.4779	0.229178
24	0.7811	1.0266	1.0687	0.0410092	2.0754	2.5971	0.251373

Table5.23 (continued)

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
25	0.8299	1.0129	1.0414	0.0281370	2.1990	2.8912	0.314779
26	0.8454	1.0119	1.0342	0.0220378	2.2319	2.9964	0.342533
27	0.8559	1.0090	1.0298	0.0206145	2.2551	3.0712	0.361891
28	0.8638	1.0067	1.0266	0.0197676	2.2808	3.1295	0.372106
29	0.8713	1.0067	1.0238	0.0169862	2.2856	3.1866	0.394207
30	0.8801	1.0063	1.0207	0.0143098	2.2957	3.2558	0.418217
31	0.8911	1.0057	1.0171	0.0113354	2.3121	3.3457	0.447039
32	0.9031	1.0051	1.0136	0.0084569	2.3094	3.4486	0.493288
33	0.9136	1.0039	1.0108	0.0068732	2.3544	3.5428	0.504757
34	0.9263	1.0035	1.0079	0.0043847	2.3644	3.6625	0.549019
35	0.9344	1.0014	1.0063	0.0048931	2.4221	3.7422	0.545023
36	0.9480	1.0011	1.0040	0.0028968	2.4432	3.8825	0.589104
37	0.9528	1.0001	1.0033	0.0031997	2.4777	3.9341	0.587803
Sum of data		53.3372	61.5201	4.2111077	64.0876	80.8443	7.643428

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1exp}}{\gamma_{1exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2exp}}{\gamma_{2exp}}\right)\right|\right]\text{x100}$$

= ((4.2111077+7.643428) x 100)/37

= 32.04%

Table5.24 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = $1.45A_{21}$.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
1	0.0874	3.4513	2.5149	0.271318054	1.0187	1.0218	0.003043
2	0.0967	3.3591	2.4161	0.280729957	1.0192	1.0260	0.006672
3	0.1411	2.8214	2.0478	0.274190118	1.0463	1.0490	0.002581
4	0.1756	2.4675	1.8445	0.252482270	1.0731	1.0698	0.003075
5	0.2065	2.2331	1.7030	0.237383010	1.0995	1.0901	0.008549
6	0.2253	2.0935	1.6310	0.220921901	1.1181	1.1031	0.013416
7	0.2252	1.9235	1.6314	0.151858591	1.1505	1.1031	0.041199
8	0.2856	1.7856	1.4518	0.186939964	1.1822	1.1478	0.029098
9	0.3133	1.6845	1.3892	0.175304245	1.2124	1.1697	0.035219
10	0.3535	1.5497	1.3141	0.152029425	1.2689	1.2026	0.052250
11	0.3773	1.4861	1.2767	0.140905726	1.2967	1.2227	0.057068
12	0.3999	1.4325	1.2453	0.130680628	1.3258	1.2422	0.063056
13	0.4258	1.3738	1.2135	0.116683651	1.3637	1.2650	0.072377
14	0.4691	1.2973	1.1686	0.099206043	1.4273	1.3042	0.086247
15	0.4987	1.2495	1.1429	0.085314126	1.4825	1.3316	0.101788
16	0.5218	1.2158	1.1252	0.074518835	1.5257	1.3534	0.112932
17	0.5421	1.195	1.1112	0.070125523	1.5551	1.3729	0.117163
18	0.5692	1.1688	1.0945	0.063569473	1.5971	1.3991	0.123975
19	0.5907	1.1436	1.0827	0.053252886	1.6439	1.4203	0.136018
20	0.6242	1.1148	1.0665	0.043326157	1.7106	1.4537	0.150181
21	0.6697	1.0817	1.0484	0.030784876	1.8037	1.5000	0.168376
22	0.6868	1.0716	1.0426	0.027062337	1.8439	1.5176	0.176962
23	0.7586	1.0366	1.0232	0.012926876	2.0159	1.5933	0.209633
24	0.7811	1.0266	1.0186	0.007792714	2.0754	1.6175	0.220632

Table5.24 (continued)

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
25	0.8299	1.0129	1.0107	0.002171981	2.1990	1.6708	0.240200
26	0.8454	1.0119	1.0087	0.003162368	2.2319	1.6879	0.243739
27	0.8559	1.0090	1.0075	0.001486620	2.2551	1.6995	0.246375
28	0.8638	1.0067	1.0066	0.000099350	2.2808	1.7083	0.251008
29	0.8713	1.0067	1.0059	0.000794676	2.2856	1.7167	0.248906
30	0.8801	1.0063	1.005	0.001291861	2.2957	1.7266	0.247898
31	0.8911	1.0057	1.0041	0.001590932	2.3121	1.7390	0.247870
32	0.9031	1.0051	1.0032	0.001890359	2.3094	1.7525	0.241145
33	0.9136	1.0039	1.0025	0.001394561	2.3544	1.7644	0.250595
34	0.9263	1.0035	1.0018	0.001694071	2.3644	1.7789	0.247632
35	0.9344	1.0014	1.0014	0.000000000	2.4221	1.7882	0.261715
36	0.9480	1.0011	1.0009	0.000199780	2.4432	1.8038	0.261706
37	0.9528	1.0001	1.0007	0.000599940	2.4777	1.8093	0.269766
Sum of data		53.3372	46.6627	3.175683871	64.0876	53.2224	5.250065

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1exp}}{\gamma_{1exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2exp}}{\gamma_{2exp}}\right)\right|\right]\text{x}100$$

= ((3.175683871+5.250065) x 100)/37

= 22.77%

Table5.25 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = 0.55A_{21}.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
1	0.0874	3.4513	4.7720	0.382667401	1.0187	1.0268	0.007951310
2	0.0967	3.3591	4.5353	0.350153315	1.0192	1.0321	0.012656986
3	0.1411	2.8214	3.6546	0.295314383	1.0463	1.0624	0.015387556
4	0.1756	2.4675	3.1685	0.284093212	1.0731	1.0913	0.016960209
5	0.2065	2.2331	2.8296	0.267117460	1.0995	1.1208	0.019372442
6	0.2253	2.0935	2.6566	0.268975400	1.1181	1.1404	0.019944549
7	0.2252	1.9235	2.6574	0.381544060	1.1505	1.1403	0.008865711
8	0.2856	1.7856	2.223	0.244959677	1.1822	1.2121	0.025291829
9	0.3133	1.6845	2.0697	0.228673197	1.2124	1.2497	0.030765424
10	0.3535	1.5497	1.8839	0.215654643	1.2689	1.3098	0.032232642
11	0.3773	1.4861	1.7904	0.204764148	1.2967	1.3488	0.040178916
12	0.3999	1.4325	1.7109	0.194345550	1.3258	1.3883	0.047141349
13	0.4258	1.3738	1.6294	0.186053283	1.3637	1.4368	0.053604165
14	0.4691	1.2973	1.5124	0.165805905	1.4273	1.5261	0.069221607
15	0.4987	1.2495	1.4438	0.155502201	1.4825	1.5939	0.075143339
16	0.5218	1.2158	1.3958	0.148050666	1.5257	1.6511	0.082191781
17	0.5421	1.195	1.3572	0.135732218	1.5551	1.7046	0.096135297
18	0.5692	1.1688	1.3102	0.120978782	1.5971	1.7814	0.115396656
19	0.5907	1.1436	1.2763	0.116037076	1.6439	1.847	0.123547661
20	0.6242	1.1148	1.2288	0.102260495	1.7106	1.9585	0.144919911
21	0.6697	1.0817	1.1736	0.084958861	1.8037	2.1308	0.181349448
22	0.6868	1.0716	1.1553	0.078107503	1.8439	2.2027	0.194587559
23	0.7586	1.0366	1.0911	0.052575728	2.0159	2.5566	0.26821767
24	0.7811	1.0266	1.0748	0.046951101	2.0754	2.6882	0.295268382

Table5.25 (continued)

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
25	0.8299	1.0129	1.0453	0.031987363	2.1990	3.0168	0.371896317
26	0.8454	1.0119	1.0375	0.025298943	2.2319	3.1355	0.404856848
27	0.8559	1.0090	1.0327	0.023488603	2.2551	3.2205	0.428096315
28	0.8638	1.0067	1.0293	0.022449588	2.2808	3.2870	0.441160996
29	0.8713	1.0067	1.0262	0.019370220	2.2856	3.3522	0.466660833
30	0.8801	1.0063	1.0228	0.016396701	2.2957	3.4316	0.494794616
31	0.8911	1.0057	1.0188	0.013025753	2.3121	3.5352	0.528999611
32	0.9031	1.0051	1.0150	0.009849766	2.3094	3.6543	0.582359054
33	0.9136	1.0039	1.0120	0.008068533	2.3544	3.7639	0.598666327
34	0.9263	1.0035	1.0087	0.005181863	2.3644	3.9040	0.651158856
35	0.9344	1.0014	1.0070	0.005592171	2.4221	3.9978	0.650551175
36	0.9480	1.0011	1.0044	0.003296374	2.4432	4.1638	0.704240341
37	0.9528	1.0001	1.0036	0.003499650	2.4777	4.2251	0.705250837
Sum of data		53.3372	62.8639	4.89878179	64.0876	83.8882	9.005024525

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1\exp}}{\gamma_{1\exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2\exp}}{\gamma_{2\exp}}\right)\right|\right]\text{x}100$$

= ((4.89878179+9.005024525) x 100)/37

= 37.58%

Table5.26 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = 1.50A_{21}.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
1	0.0874	3.4513	2.4328	0.2951062	1.0187	1.0215	0.002749
2	0.0967	3.3591	2.3391	0.3036528	1.0192	1.0255	0.006181
3	0.1411	2.8214	1.9898	0.2947473	1.0463	1.0480	0.001625
4	0.1756	2.4675	1.7970	0.2717325	1.0731	1.0682	0.004566
5	0.2065	2.2331	1.6629	0.2553401	1.0995	1.0879	0.010550
6	0.2253	2.0935	1.5947	0.2382613	1.1181	1.1006	0.015652
7	0.2252	1.9235	1.5950	0.1707824	1.1505	1.1005	0.043459
8	0.2856	1.7856	1.4250	0.2019489	1.1822	1.1437	0.032566
9	0.3133	1.6845	1.3657	0.1892550	1.2124	1.1646	0.039426
10	0.3535	1.5497	1.2947	0.1645480	1.2689	1.1961	0.057373
11	0.3773	1.4861	1.2594	0.1525469	1.2967	1.2152	0.062852
12	0.3999	1.4325	1.2298	0.1415009	1.3258	1.2338	0.069392
13	0.4258	1.3738	1.1997	0.1267288	1.3637	1.2554	0.079416
14	0.4691	1.2973	1.1575	0.1077623	1.4273	1.2923	0.094584
15	0.4987	1.2495	1.1333	0.0929972	1.4825	1.3181	0.110894
16	0.5218	1.2158	1.1167	0.0815101	1.5257	1.3385	0.122698
17	0.5421	1.1950	1.1035	0.0765690	1.5551	1.3367	0.140441
18	0.5692	1.1688	1.0879	0.0692163	1.5971	1.3812	0.135183
19	0.5907	1.1436	1.0768	0.0584120	1.6439	1.4008	0.147880
20	0.6242	1.1148	1.0617	0.0476319	1.7106	1.4317	0.163042
21	0.6697	1.0817	1.0448	0.0341130	1.8037	1.4744	0.182569
22	0.6868	1.0716	1.0394	0.0300485	1.8439	1.4906	0.191605
23	0.7586	1.0366	1.0214	0.0146633	2.0159	1.5597	0.226301
24	0.7811	1.0266	1.0172	0.0091564	2.0754	1.5816	0.237930

Table5.26(continued)

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
25	0.8299	1.0129	1.0098	0.0030605	2.1990	1.6297	0.258890
26	0.8454	1.0119	1.0080	0.0038541	2.2319	1.6451	0.262915
27	0.8559	1.0090	1.0068	0.0021804	2.2551	1.6556	0.265842
28	0.8638	1.0067	1.0061	0.0005960	2.2808	1.6635	0.270651
29	0.8713	1.0067	1.0054	0.0012913	2.2856	1.6710	0.268901
30	0.8801	1.0063	1.0046	0.0016894	2.2957	1.6799	0.268241
31	0.8911	1.0057	1.0038	0.0018892	2.3121	1.6909	0.268674
32	0.9031	1.0051	1.0029	0.0021888	2.3094	1.7030	0.262579
33	0.9136	1.0039	1.0023	0.0015938	2.3544	1.7136	0.272171
34	0.9263	1.0035	1.0017	0.0017937	2.3644	1.7265	0.269794
35	0.9344	1.0014	1.0013	0.0000999	2.4221	1.7348	0.283762
36	0.9480	1.0011	1.0008	0.0002997	2.4432	1.7486	0.284299
37	0.9528	1.0001	1.0007	0.0005999	2.4777	1.7535	0.292287
Sum of data		53.3372	46.1	3.4493679	64.0876	52.2823	5.707939

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1\exp}}{\gamma_{1\exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2\exp}}{\gamma_{2\exp}}\right)\right|\right]\text{x}100$$

= ((3.4493679+5.707939) x 100)/37

= 24.75%

Table5.27 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = 0.50A_{21}.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
1	0.0874	3.4513	4.9577	0.4364732	1.0187	1.0269	0.008049
2	0.0967	3.3591	4.7101	0.4021911	1.0192	1.0323	0.012853
3	0.1411	2.8214	3.7888	0.3428794	1.0463	1.0629	0.015865
4	0.1756	2.4675	3.2804	0.3294428	1.0731	1.0920	0.017613
5	0.2065	2.2331	2.9257	0.3101518	1.0995	1.1219	0.020373
6	0.2253	2.0935	2.7447	0.3110580	1.1181	1.1418	0.021197
7	0.2252	1.9235	2.7456	0.4273980	1.1505	1.1417	0.007649
8	0.2856	1.7856	2.2908	0.2829301	1.1822	1.2147	0.027491
9	0.3133	1.6845	2.1303	0.2646483	1.2124	1.2530	0.033487
10	0.3535	1.5497	1.9356	0.2490159	1.2689	1.3144	0.035858
11	0.3773	1.4861	1.8375	0.2364578	1.2967	1.3544	0.044498
12	0.3999	1.4325	1.754	0.2244328	1.3258	1.3950	0.052195
13	0.4258	1.3738	1.6685	0.2145145	1.3637	1.4449	0.059544
14	0.4691	1.2973	1.5454	0.1912434	1.4273	1.5374	0.077139
15	0.4987	1.2495	1.4733	0.1791116	1.4825	1.6078	0.084519
16	0.5218	1.2158	1.4227	0.1701760	1.5257	1.6674	0.092875
17	0.5421	1.1950	1.3819	0.1564017	1.5551	1.7234	0.108225
18	0.5692	1.1688	1.3323	0.1398871	1.5971	1.8041	0.129610
19	0.5907	1.1436	1.2964	0.1336132	1.6439	1.8733	0.139546
20	0.6242	1.1148	1.2461	0.1177790	1.7106	1.9916	0.164270
21	0.6697	1.0817	1.1874	0.0977166	1.8037	2.1758	0.206298
22	0.6868	1.0716	1.1679	0.0898656	1.8439	2.2532	0.221975
23	0.7586	1.0366	1.0992	0.0603897	2.0159	2.6391	0.309142
24	0.7811	1.0266	1.0817	0.0536723	2.0754	2.7845	0.341669

Table5.27 (continued)

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
25	0.8299	1.0129	1.0498	0.0364301	2.1990	3.1524	0.433561
26	0.8454	1.0119	1.0413	0.0290543	2.2319	3.2871	0.472781
27	0.8559	1.0090	1.036	0.0267592	2.2551	3.3839	0.500554
28	0.8638	1.0067	1.0323	0.0254296	2.2808	3.4600	0.517012
29	0.8713	1.0067	1.0289	0.0220522	2.2856	3.5349	0.546596
30	0.8801	1.0063	1.0252	0.0187817	2.2957	3.6264	0.579649
31	0.8911	1.0057	1.0209	0.0151139	2.3121	3.7465	0.620388
32	0.9031	1.0051	1.0166	0.0114416	2.3094	3.8852	0.682342
33	0.9136	1.0039	1.0133	0.0093635	2.3544	4.0138	0.704808
34	0.9263	1.0035	1.0097	0.0061784	2.3644	4.1790	0.767467
35	0.9344	1.0014	1.0078	0.0063911	2.4221	4.2904	0.771355
36	0.9480	1.0011	1.0049	0.0037958	2.4432	4.4887	0.837222
37	0.9528	1.0001	1.0041	0.0039996	2.4777	4.5624	0.841385
Sum of data		53.3372	64.2948	5.6362407	64.0876	87.2642	10.50706

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1exp}}{\gamma_{1exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2exp}}{\gamma_{2exp}}\right)\right|\right]x100$$

= ((5.6362407+10.50706) x 100)/37

= 43.63%

Table5.28 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = 1.60A_{21}.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
1	0.0874	3.4513	2.2781	0.339929881	1.0187	1.0207	0.001963
2	0.0967	3.3591	2.1940	0.346848858	1.0192	1.0246	0.005298
3	0.1411	2.8214	1.8805	0.333486921	1.0463	1.0460	0.000287
4	0.1756	2.4675	1.7076	0.307963526	1.0731	1.0651	0.007455
5	0.2065	2.2331	1.5872	0.289239174	1.0995	1.0836	0.014461
6	0.2253	2.0935	1.5262	0.27098161	1.1181	1.0953	0.020392
7	0.2252	1.9235	1.5265	0.206394593	1.1505	1.0953	0.047979
8	0.2856	1.7856	1.3743	0.230342742	1.1822	1.1352	0.039756
9	0.3133	1.6845	1.3214	0.215553577	1.2124	1.1544	0.047839
10	0.3535	1.5497	1.2582	0.188100923	1.2689	1.1830	0.067696
11	0.3773	1.4861	1.2268	0.174483548	1.2967	1.2003	0.074343
12	0.3999	1.4325	1.2005	0.161954625	1.3258	1.2170	0.082064
13	0.4258	1.3738	1.1739	0.145508808	1.3637	1.2363	0.093422
14	0.4691	1.2973	1.1366	0.123872659	1.4273	1.2690	0.110909
15	0.4987	1.2495	1.1153	0.107402961	1.4825	1.2917	0.128702
16	0.5218	1.2158	1.1008	0.094587926	1.5257	1.3095	0.141705
17	0.5421	1.1950	1.0892	0.088535565	1.5551	1.3252	0.147836
18	0.5692	1.1688	1.0755	0.079825462	1.5971	1.3463	0.157035
19	0.5907	1.1436	1.0659	0.067943337	1.6439	1.3632	0.170752
20	0.6242	1.1148	1.0528	0.055615357	1.7106	1.3896	0.187653
21	0.6697	1.0817	1.0381	0.040306924	1.8037	1.4256	0.209625
22	0.6868	1.0716	1.0335	0.035554311	1.8439	1.4391	0.219535
23	0.7586	1.0366	1.0181	0.017846807	2.0159	1.4964	0.257701
24	0.7811	1.0266	1.0145	0.011786480	2.0754	1.5144	0.270309

Table5.28 (continued)

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
25	0.8299	1.0129	1.0082	0.004640142	2.1990	1.5534	0.293588
26	0.8454	1.0119	1.0067	0.005138848	2.2319	1.5658	0.298445
27	0.8559	1.0090	1.0057	0.003270565	2.2551	1.5742	0.301938
28	0.8638	1.0067	1.0051	0.001589351	2.2808	1.5805	0.307041
29	0.8713	1.0067	1.0045	0.002185358	2.2856	1.5865	0.305872
30	0.8801	1.0063	1.0039	0.002384975	2.2957	1.5936	0.305833
31	0.8911	1.0057	1.0031	0.002585264	2.3121	1.6024	0.306950
32	0.9031	1.0051	1.0025	0.002586807	2.3094	1.6120	0.301983
33	0.9136	1.0039	1.0019	0.001992230	2.3544	1.6204	0.311757
34	0.9263	1.0035	1.0014	0.002092676	2.3644	1.6305	0.310396
35	0.9344	1.0014	1.0011	0.000299581	2.4221	1.6370	0.324140
36	0.9480	1.0011	1.0007	0.000399560	2.4432	1.6478	0.325557
37	0.9528	1.0001	1.0006	0.000499950	2.4777	1.6517	0.333374
Sum of data		53.3372	45.0409	3.963731881	64.0876	50.5826	6.531591

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1\exp}}{\gamma_{1\exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2\exp}}{\gamma_{2\exp}}\right)\right|\right]\text{x}100$$

$$= ((3.963731881+6.531591) \text{ x } 100)/37$$

$$= 28.37\%$$

Table5.29 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = 0.40A_{21}.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
1	0.0874	3.4513	5.3556	0.5517631	1.0187	1.0272	0.008344
2	0.0967	3.3591	5.0850	0.5137983	1.0192	1.0326	0.013148
3	0.1411	2.8214	4.0779	0.4453463	1.0463	1.0637	0.016630
4	0.1756	2.4675	3.5221	0.4273961	1.0731	1.0934	0.018917
5	0.2065	2.2331	3.1342	0.4035198	1.0995	1.1239	0.022192
6	0.2253	2.0935	2.9361	0.4024839	1.1181	1.1442	0.023343
7	0.2252	1.9235	2.9371	0.5269561	1.1505	1.1441	0.005563
8	0.2856	1.7856	2.4392	0.3660394	1.1822	1.2192	0.031298
9	0.3133	1.6845	2.2632	0.3435441	1.2124	1.2589	0.038354
10	0.3535	1.5497	2.0494	0.3224495	1.2689	1.3228	0.042478
11	0.3773	1.4861	1.9416	0.3065070	1.2967	1.3646	0.052364
12	0.3999	1.4325	1.8498	0.2913089	1.3258	1.4073	0.061472
13	0.4258	1.3738	1.7555	0.2778425	1.3637	1.4600	0.070617
14	0.4691	1.2973	1.6196	0.2484391	1.4273	1.5584	0.091852
15	0.4987	1.2495	1.5397	0.2322529	1.4825	1.6341	0.102260
16	0.5218	1.2158	1.4836	0.2202665	1.5257	1.6986	0.113325
17	0.5421	1.195	1.4382	0.2035146	1.5551	1.7597	0.131567
18	0.5692	1.1688	1.3828	0.1830938	1.5971	1.8482	0.157222
19	0.5907	1.1436	1.3427	0.1740993	1.6439	1.9249	0.170935
20	0.6242	1.1148	1.2862	0.1537496	1.7106	2.0573	0.202677
21	0.6697	1.0817	1.2198	0.1276694	1.8037	2.2672	0.256972
22	0.6868	1.0716	1.1976	0.1175812	1.8439	2.3567	0.278106
23	0.7586	1.0366	1.1187	0.0792012	2.0159	2.8152	0.396498
24	0.7811	1.0266	1.0984	0.0699396	2.0754	2.9935	0.442373

Table5.29 (continued)

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\vert(\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp}\vert$	γ_{2exp}	γ_{2exp}	$\vert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\vert$
25	0.8299	1.0129	1.0609	0.0473887	2.1990	3.4579	0.572487
26	0.8454	1.0119	1.0508	0.0384425	2.2319	3.6328	0.627671
27	0.8559	1.0090	1.0444	0.0350842	2.2551	3.7603	0.667465
28	0.8638	1.0067	1.0399	0.0329790	2.2808	3.8614	0.693002
29	0.8713	1.0067	1.0358	0.0289063	2.2856	3.9619	0.733418
30	0.8801	1.0063	1.0313	0.0248435	2.2957	4.0857	0.779719
31	0.8911	1.0057	1.0261	0.0202844	2.3121	4.2501	0.838199
32	0.9031	1.0051	1.0209	0.0157198	2.3094	4.4428	0.923790
33	0.9136	1.0039	1.0168	0.0128499	2.3544	4.6241	0.964025
34	0.9263	1.0035	1.0124	0.0088690	2.3644	4.8609	1.055870
35	0.9344	1.0014	1.0099	0.0084881	2.4221	5.0229	1.073779
36	0.9480	1.0011	1.0063	0.0051943	2.4432	5.3164	1.175999
37	0.9528	1.0001	1.0052	0.0050995	2.4777	5.4300	1.191549
Sum of data		53.3372	67.4347	7.2729114	64.0876	95.2829	14.04548

N = number of data points

%Average Absolute Deviation = $\frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1exp}}{\gamma_{1exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2exp}}{\gamma_{2exp}}\right)\right|\right]$x100

= ((7.2729114+14.04548) x 100)/37

= 57.62%

Table5.30 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = 1.70A_{21}.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert (\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp} \rvert$	γ_{2exp}	γ_{2exp}	$\lvert (\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp} \rvert$
1	0.0874	3.4513	2.1353	0.3813056	1.0187	1.0198	0.001080
2	0.0967	3.3591	2.0600	0.3867405	1.0192	1.0236	0.004317
3	0.1411	2.8214	1.7795	0.3692848	1.0463	1.0438	0.002389
4	0.1756	2.4675	1.6248	0.3415198	1.0731	1.0618	0.010530
5	0.2065	2.2331	1.5173	0.3205410	1.0995	1.0790	0.018645
6	0.2253	2.0935	1.4628	0.3012658	1.1181	1.0900	0.025132
7	0.2252	1.9235	1.4631	0.2393553	1.1505	1.0899	0.052673
8	0.2856	1.7856	1.3275	0.2565524	1.1822	1.1267	0.046946
9	0.3133	1.6845	1.2805	0.2398338	1.2124	1.1441	0.056335
10	0.3535	1.5497	1.2245	0.2098471	1.2689	1.1700	0.077942
11	0.3773	1.4861	1.1968	0.1946706	1.2967	1.1855	0.085756
12	0.3999	1.4325	1.1736	0.1807330	1.3258	1.2003	0.094660
13	0.4258	1.3738	1.1502	0.1627602	1.3637	1.2174	0.107282
14	0.4691	1.2973	1.1174	0.1386726	1.4273	1.2462	0.126883
15	0.4987	1.2495	1.0989	0.1205282	1.4825	1.2659	0.146105
16	0.5218	1.2158	1.0862	0.1065965	1.5257	1.2813	0.160189
17	0.5421	1.1950	1.0762	0.0994142	1.5551	1.2949	0.167320
18	0.5692	1.1688	1.0643	0.0894079	1.5971	1.3130	0.177885
19	0.5907	1.1436	1.0559	0.0766877	1.6439	1.3273	0.192591
20	0.6242	1.1148	1.0446	0.0629709	1.7106	1.3496	0.211037
21	0.6697	1.0817	1.0321	0.0458537	1.8037	1.3797	0.235072
22	0.6868	1.0716	1.0281	0.0405935	1.8439	1.3909	0.245675
23	0.7586	1.0366	1.0151	0.0207409	2.0159	1.4379	0.286721
24	0.7811	1.0266	1.0120	0.0142217	2.0754	1.4544	0.299219

Table5.30 (continued)

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
25	0.8299	1.0129	1.0068	0.0060223	2.1990	1.4838	0.325239
26	0.8454	1.0119	1.0055	0.0063247	2.2319	1.4937	0.330750
27	0.8559	1.0090	1.0047	0.0042616	2.2551	1.5003	0.334708
28	0.8638	1.0067	1.0042	0.0024834	2.2808	1.5054	0.339968
29	0.8713	1.0067	1.0037	0.0029800	2.2856	1.5101	0.339298
30	0.8801	1.0063	1.0032	0.0030806	2.2957	1.5156	0.339809
31	0.8911	1.0057	1.0026	0.0030824	2.3121	1.5226	0.341464
32	0.9031	1.0051	1.0020	0.0030843	2.3094	1.5301	0.337447
33	0.9136	1.0039	1.0016	0.0022911	2.3544	1.5367	0.347307
34	0.9263	1.0035	1.0011	0.0023916	2.3644	1.5446	0.346726
35	0.9344	1.0014	1.0009	0.0004993	2.4221	1.5496	0.360225
36	0.9480	1.0011	1.0005	0.0005993	2.4432	1.5581	0.362271
37	0.9528	1.0001	1.0005	0.0004000	2.4777	1.5610	0.369980
Sum of data		53.3372	44.064	4.4375984	64.0876	49.0046	7.307576

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1exp}}{\gamma_{1exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2exp}}{\gamma_{2exp}}\right)\right|\right]x100$$

= ((4.4375984+7.307576) x 100)/37

= 31.74%

Table5.31 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = 0.30A_{21}.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
1	0.0874	3.4513	5.7925	0.6783531	1.0187	1.0274	0.008540
2	0.0967	3.3591	5.4970	0.6364502	1.0192	1.0329	0.013442
3	0.1411	2.8214	4.3976	0.5586588	1.0463	1.0643	0.017203
4	0.1756	2.4675	3.7906	0.5362107	1.0731	1.0944	0.019849
5	0.2065	2.2331	3.3669	0.5077247	1.0995	1.1254	0.023556
6	0.2253	2.0935	3.1505	0.5048961	1.1181	1.1462	0.025132
7	0.2252	1.9235	3.1515	0.6384195	1.1505	1.1461	0.003820
8	0.2856	1.7856	2.6070	0.4600134	1.1822	1.2230	0.034512
9	0.3133	1.6845	2.4142	0.4331849	1.2124	1.2638	0.042395
10	0.3535	1.5497	2.1799	0.4066594	1.2689	1.3299	0.048073
11	0.3773	1.4861	2.0616	0.3872552	1.2967	1.3734	0.059150
12	0.3999	1.4325	1.9607	0.3687260	1.3258	1.4179	0.069467
13	0.4258	1.3738	1.8569	0.3516524	1.3637	1.4731	0.080223
14	0.4691	1.2973	1.7070	0.3158098	1.4273	1.5770	0.104883
15	0.4987	1.2495	1.6186	0.2953982	1.4825	1.6577	0.118179
16	0.5218	1.2158	1.5563	0.2800625	1.5257	1.7268	0.131808
17	0.5421	1.1950	1.5058	0.2600837	1.5551	1.7927	0.152788
18	0.5692	1.1688	1.4441	0.2355407	1.5971	1.8891	0.182831
19	0.5907	1.1436	1.3992	0.2235047	1.6439	1.9732	0.200316
20	0.6242	1.1148	1.3358	0.1982418	1.7106	2.2102	0.292061
21	0.6697	1.0817	1.2607	0.1654803	1.8037	2.3575	0.307036
22	0.6868	1.0716	1.2354	0.1528555	1.8439	2.4604	0.334346
23	0.7586	1.0366	1.1445	0.1040903	2.0159	3.0037	0.490004
24	0.7811	1.0266	1.1207	0.0916618	2.0754	3.2225	0.552713

Table5.31 (continued)

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
25	0.8299	1.0129	1.0761	0.0623951	2.1990	3.8137	0.734288
26	0.8454	1.0119	1.0640	0.0514873	2.2319	4.0445	0.812133
27	0.8559	1.0090	1.0563	0.0468781	2.2551	4.2155	0.869318
28	0.8638	1.0067	1.0507	0.0437072	2.2808	4.3529	0.908497
29	0.8713	1.0067	1.0458	0.0388398	2.2856	4.4910	0.964911
30	0.8801	1.0063	1.0402	0.0336878	2.2957	4.6633	1.031319
31	0.8911	1.0057	1.0337	0.0278413	2.3121	4.8958	1.117469
32	0.9031	1.0051	1.0271	0.0218884	2.3094	5.1739	1.240365
33	0.9136	1.0039	1.0219	0.0179301	2.3544	5.4409	1.310950
34	0.9263	1.0035	1.0163	0.0127554	2.3644	5.7977	1.452081
35	0.9344	1.0014	1.0131	0.0116836	2.4221	6.0472	1.496676
36	0.9480	1.0011	1.0084	0.0072920	2.4432	6.5106	1.664784
37	0.9528	1.0001	1.007	0.0068993	2.4777	6.6890	1.699681
Sum of data		53.3372	64.0876	9.1742191	64.0876	105.725	18.61481

N = number of data points

$$\%\text{Average Absolute Deviation} = \tfrac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1\exp}}{\gamma_{1\exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2\exp}}{\gamma_{2\exp}}\right)\right|\right]x100$$

= ((9.1742191+18.61481) x 100)/37

= 75.11%

Table5.32 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = 1.80A_{21}.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
1	0.0874	3.4513	2.0032	0.4195810	1.0187	1.0190	0.000294
2	0.0967	3.3591	1.9360	0.4236551	1.0192	1.0225	0.003238
3	0.1411	2.8214	1.6859	0.4024598	1.0463	1.0416	0.004492
4	0.1756	2.4675	1.5481	0.3726039	1.0731	1.0584	0.013699
5	0.2065	2.2331	1.4525	0.3495589	1.0995	1.0744	0.022829
6	0.2253	2.0935	1.404	0.3293528	1.1181	1.0845	0.030051
7	0.2252	1.9235	1.4043	0.2699246	1.1505	1.0845	0.057366
8	0.2856	1.7856	1.2842	0.2808020	1.1822	1.1180	0.054306
9	0.3133	1.6845	1.2427	0.2622737	1.2124	1.1338	0.064830
10	0.3535	1.5497	1.1933	0.2299800	1.2689	1.1570	0.088187
11	0.3773	1.4861	1.1690	0.2133773	1.2967	1.1708	0.097093
12	0.3999	1.4325	1.1487	0.1981152	1.3258	1.1839	0.107030
13	0.4258	1.3738	1.1283	0.1787014	1.3637	1.1989	0.120848
14	0.4691	1.2973	1.0997	0.1523163	1.4273	1.2239	0.142507
15	0.4987	1.2495	1.0837	0.1326931	1.4825	1.2410	0.162901
16	0.5218	1.2158	1.0727	0.1177003	1.5257	1.2542	0.177951
17	0.5421	1.195	1.0641	0.1095397	1.5551	1.2657	0.186097
18	0.5692	1.1688	1.0540	0.0982204	1.5971	1.2810	0.197921
19	0.5907	1.1436	1.0468	0.0846450	1.6439	1.2930	0.213456
20	0.6242	1.1148	1.0372	0.0696089	1.7106	1.3116	0.233251
21	0.6697	1.0817	1.0266	0.0509383	1.8037	1.3365	0.259023
22	0.6868	1.0716	1.0233	0.0450728	1.8439	1.3457	0.270188
23	0.7586	1.0366	1.0124	0.0233456	2.0159	1.3837	0.313607
24	0.7811	1.0266	1.0098	0.0163647	2.0754	1.3953	0.327696

Table5.32 (continued)

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
25	0.8299	1.0129	1.0055	0.0073058	2.1990	1.4201	0.354206
26	0.8454	1.0119	1.0045	0.0073130	2.2319	1.4279	0.360231
27	0.8559	1.0090	1.0038	0.0051536	2.2551	1.4331	0.364507
28	0.8638	1.0067	1.0034	0.0032780	2.2808	1.4370	0.369958
29	0.8713	1.0067	1.0030	0.0036754	2.2856	1.4401	0.369925
30	0.8801	1.0063	1.0026	0.0036768	2.2957	1.4450	0.370562
31	0.8911	1.0057	1.0021	0.0035796	2.3121	1.4503	0.372735
32	0.9031	1.0051	1.0016	0.0034822	2.3094	1.4561	0.369490
33	0.9136	1.0039	1.0013	0.0025899	2.3544	1.4612	0.379375
34	0.9263	1.0035	1.0009	0.0025909	2.3644	1.4673	0.379420
35	0.9344	1.0014	1.0007	0.0006990	2.4221	1.4711	0.392634
36	0.9480	1.0011	1.0004	0.0006992	2.4432	1.4775	0.395260
37	0.9528	1.0001	1.0004	0.0003000	2.4777	1.4798	0.402753
Sum of data		53.3372	43.1607	4.8751742	64.0876	47.5454	8.029916

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1exp}}{\gamma_{1exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2exp}}{\gamma_{2exp}}\right)\right|\right]\text{x}100$$

= ((4.8751742+8.029916) x 100)/37

= 34.85%

Table5.33 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = $0.20A_{21}$.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert (\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp} \rvert$	γ_{2exp}	γ_{2exp}	$\lvert (\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp} \rvert$
1	0.0874	3.4513	6.2726	0.817460088	1.0187	1.0276	0.0087366
2	0.0967	3.3591	5.9505	0.771456640	1.0192	1.0331	0.0136381
3	0.1411	2.8214	4.7518	0.684199334	1.0463	1.0648	0.0176814
4	0.1756	2.4675	4.0898	0.657467072	1.0731	1.0952	0.0205945
5	0.2065	2.2331	3.6276	0.624468228	1.0995	1.1266	0.0246476
6	0.2253	2.0935	3.3914	0.619966563	1.1181	1.1477	0.0264735
7	0.2252	1.9235	3.3926	0.763763972	1.1505	1.1476	0.0025206
8	0.2856	1.7856	2.7978	0.56686828	1.1822	1.2258	0.0368804
9	0.3133	1.6845	2.5871	0.535826655	1.2124	1.2675	0.0454470
10	0.3535	1.5497	2.3307	0.50396851	1.2689	1.3354	0.0524076
11	0.3773	1.4861	2.2010	0.481057802	1.2967	1.3802	0.0643942
12	0.3999	1.4325	2.0903	0.459197208	1.3258	1.4262	0.0757279
13	0.4258	1.3738	1.9763	0.438564565	1.3637	1.4836	0.0879226
14	0.4691	1.2973	1.8111	0.396053342	1.4273	1.5921	0.1154628
15	0.4987	1.2495	1.7135	0.371348539	1.4825	1.6770	0.1311973
16	0.5218	1.2158	1.6446	0.352689587	1.5257	1.7504	0.1472767
17	0.5421	1.1950	1.5886	0.329372385	1.5551	1.8206	0.1707286
18	0.5692	1.1688	1.5199	0.300393566	1.5971	1.9241	0.2047461
19	0.5907	1.1436	1.4698	0.285239594	1.6439	2.0153	0.2259262
20	0.6242	1.1148	1.3986	0.254574812	1.7106	2.1762	0.2721852
21	0.6697	1.0817	1.3137	0.214477212	1.8037	2.4410	0.3533293
22	0.6868	1.0716	1.2849	0.199048152	1.8439	2.5578	0.3871685
23	0.7586	1.0366	1.1801	0.13843334	2.0159	3.1954	0.5850985
24	0.7811	1.0266	1.1521	0.122248198	2.0754	3.4629	0.6685458

Table5.33 (continued)

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
25	0.8299	1.0129	1.0987	0.084707276	2.1990	4.2177	0.9180082
26	0.8454	1.0119	1.0838	0.071054452	2.2319	4.5258	1.0277790
27	0.8559	1.0090	1.0742	0.064618434	2.2551	4.7594	1.1105051
28	0.8638	1.0067	1.0674	0.060296017	2.2808	4.9504	1.1704665
29	0.8713	1.0067	1.0611	0.054037946	2.2856	5.1452	1.2511376
30	0.8801	1.0063	1.0540	0.047401371	2.2957	5.3925	1.3489567
31	0.8911	1.0057	1.0457	0.039773292	2.3121	5.7339	1.4799533
32	0.9031	1.0051	1.0373	0.032036613	2.3094	6.1541	1.6648047
33	0.9136	1.0039	1.0305	0.026496663	2.3544	6.5701	1.7905624
34	0.9263	1.0035	1.0230	0.019431988	2.3644	7.1458	2.0222467
35	0.9344	1.0014	1.0186	0.017175954	2.4221	7.5625	2.1222906
36	0.9480	1.0011	1.0122	0.011087803	2.4432	8.3679	2.4249754
37	0.9528	1.0001	1.0102	0.01009899	2.4777	8.6894	2.5070428
Sum of data		53.3372	75.1531	11.42636044	64.0876	119.589	24.57747

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1\exp}}{\gamma_{1\exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2\exp}}{\gamma_{2\exp}}\right)\right|\right]x100$$

= ((24.57747+11.42636044) x 100)/37

= 97.31%

Table5.34 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = 1.90A_{21}.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert (\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp} \rvert$	γ_{2exp}	γ_{2exp}	$\lvert (\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp} \rvert$
1	0.0874	3.4513	1.8801	0.4552487	1.0187	1.0181	0.000589
2	0.0967	3.3591	1.8212	0.4578310	1.0192	1.0214	0.002159
3	0.1411	2.8214	1.5991	0.4332246	1.0463	1.0394	0.006595
4	0.1756	2.4675	1.4769	0.4014590	1.0731	1.0550	0.016867
5	0.2065	2.2331	1.3923	0.3765169	1.0995	1.0697	0.027103
6	0.2253	2.0935	1.3495	0.3553857	1.1181	1.0790	0.034970
7	0.2252	1.9235	1.3497	0.2983104	1.1505	1.0789	0.062234
8	0.2856	1.7856	1.2439	0.3033714	1.1822	1.1093	0.061665
9	0.3133	1.6845	1.2075	0.2831701	1.2124	1.1235	0.073326
10	0.3535	1.5497	1.1644	0.2486288	1.2689	1.1441	0.098353
11	0.3773	1.4861	1.1433	0.2306709	1.2967	1.1562	0.108352
12	0.3999	1.4325	1.1256	0.2142408	1.3258	1.1677	0.119249
13	0.4258	1.3738	1.1080	0.1934779	1.3637	1.1807	0.134194
14	0.4691	1.2973	1.0835	0.1648038	1.4273	1.2022	0.157710
15	0.4987	1.2495	1.0697	0.1438976	1.4825	1.2167	0.179292
16	0.5218	1.2158	1.0604	0.1278171	1.5257	1.2279	0.195189
17	0.5421	1.1950	1.0531	0.1187448	1.5551	1.2376	0.204167
18	0.5692	1.1688	1.0444	0.1064339	1.5971	1.2503	0.217144
19	0.5907	1.1436	1.0385	0.0919028	1.6439	1.2603	0.233348
20	0.6242	1.1148	1.0304	0.0757086	1.7106	1.2756	0.254297
21	0.6697	1.0817	1.0216	0.0555607	1.8037	1.2958	0.281588
22	0.6868	1.0716	1.0188	0.0492721	1.8439	1.3032	0.293237
23	0.7586	1.0366	1.0099	0.0257573	2.0159	1.3333	0.338608
24	0.7811	1.0266	1.0078	0.0183129	2.0754	1.3424	0.353185

Table5.34 (continued)

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/ \gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
25	0.8299	1.0129	1.0044	0.0083917	2.1990	1.3616	0.380809
26	0.8454	1.0119	1.0035	0.0083012	2.2319	1.3676	0.387249
27	0.8559	1.0090	1.0030	0.0059465	2.2551	1.3715	0.391823
28	0.8638	1.0067	1.0027	0.0039734	2.2808	1.3745	0.397361
29	0.8713	1.0067	1.0023	0.0043707	2.2856	1.3773	0.397401
30	0.8801	1.0063	1.0020	0.0042731	2.2957	1.3806	0.398615
31	0.8911	1.0057	1.0016	0.0040768	2.3121	1.3846	0.401150
32	0.9031	1.0051	1.0013	0.0037807	2.3094	1.3890	0.398545
33	0.9136	1.0039	1.0010	0.0028887	2.3544	1.3928	0.408427
34	0.9263	1.0035	1.0008	0.0026906	2.3644	1.3973	0.409026
35	0.9344	1.0014	1.0006	0.0007989	2.4221	1.4002	0.421907
36	0.9480	1.0011	1.0003	0.0007991	2.4432	1.4049	0.424975
37	0.9528	1.0001	1.0003	0.0002000	2.4777	1.4066	0.432296
Sum of data		53.3372	42.3234	5.2802392	64.0876	46.1968	8.703001

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1exp}}{\gamma_{1exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2exp}}{\gamma_{2exp}}\right)\right|\right]\text{x}100$$

= ((5.2805392+8.703001) x 100)/37

= 37.79%

Table5.35 The activity coefficient of ethanol(1)+water(2) at Wilson parameter = $0.10A_{21}$.

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
1	0.0874	3.4513	6.8010	0.9705618	1.0187	1.0277	0.0088348
2	0.0967	3.3591	6.4504	0.9202763	1.0192	1.0332	0.0137363
3	0.1411	2.8214	5.1452	0.8236337	1.0463	1.0651	0.0179681
4	0.1756	2.4675	4.4243	0.7930294	1.0731	1.0957	0.0210605
5	0.2065	2.2331	3.9208	0.7557655	1.0995	1.1274	0.0253752
6	0.2253	2.0935	3.6634	0.7498925	1.1181	1.1486	0.0272784
7	0.2252	1.9235	3.6647	0.9052249	1.1505	1.1485	0.0017384
8	0.2856	1.7856	3.0163	0.6892361	1.1822	1.2276	0.0384030
9	0.3133	1.6845	2.7864	0.6541407	1.2124	1.2700	0.0475091
10	0.3535	1.5497	2.5063	0.6172808	1.2689	1.3390	0.0552447
11	0.3773	1.4861	2.3645	0.5910773	1.2967	1.3847	0.0678646
12	0.3999	1.4325	2.2434	0.5660733	1.3258	1.4317	0.0798763
13	0.4258	1.3738	2.1185	0.5420731	1.3637	1.4906	0.0930557
14	0.4691	1.2973	1.9373	0.4933323	1.4273	1.6025	0.1227492
15	0.4987	1.2495	1.8299	0.4645058	1.4825	1.6905	0.1403035
16	0.5218	1.2158	1.7538	0.4425070	1.5257	1.7670	0.1581569
17	0.5421	1.1950	1.6920	0.4158996	1.5551	1.8405	0.1835252
18	0.5692	1.1688	1.6159	0.3825291	1.5971	1.9496	0.2207125
19	0.5907	1.1436	1.5602	0.3642882	1.6439	2.0463	0.2447837
20	0.6242	1.1148	1.4808	0.3283100	1.7106	2.2186	0.2969718
21	0.6697	1.0817	1.3854	0.2807618	1.8037	2.5071	0.3899762
22	0.6868	1.0716	1.3527	0.262318	1.8439	2.6363	0.4297413
23	0.7586	1.0366	1.2322	0.1886938	2.0159	3.3657	0.6695769
24	0.7811	1.0266	1.1993	0.1682252	2.0754	3.6847	0.7754168

Table5.35 (continued)

Number	Mole fraction (x_1)	γ_{1exp}	γ_{1cal}	$\lvert(\gamma_{1cal} - \gamma_{1exp})/\gamma_{1exp}\rvert$	γ_{2exp}	γ_{2exp}	$\lvert(\gamma_{2cal} - \gamma_{2exp})/\gamma_{2exp}\rvert$
25	0.8299	1.0129	1.1351	0.1206437	2.1990	4.6323	1.1065484
26	0.8454	1.0119	1.1167	0.1035675	2.2319	5.0408	1.2585241
27	0.8559	1.0090	1.1047	0.0948464	2.2551	5.3596	1.3766574
28	0.8638	1.0067	1.0960	0.0887057	2.2808	5.6263	1.4668099
29	0.8713	1.0067	1.0880	0.0807589	2.2856	5.9041	1.5831729
30	0.8801	1.0063	1.0788	0.0720461	2.2957	6.2656	1.7292765
31	0.8911	1.0057	1.0679	0.0618475	2.3121	6.7814	1.9330046
32	0.9031	1.0051	1.0565	0.0511392	2.3094	7.4444	2.2235213
33	0.9136	1.0039	1.0471	0.0430322	2.3544	8.1334	2.4545532
34	0.9263	1.0035	1.0365	0.0328849	2.3644	9.1446	2.8676197
35	0.9344	1.0014	1.0302	0.0287597	2.4221	9.9211	3.0960737
36	0.948	1.0011	1.0206	0.0194786	2.4432	11.539	3.7229044
37	0.9528	1.0001	1.0175	0.0173983	2.4777	12.2314	3.9365944
Sum of data		53.3372	80.0403	14.184745	64.0876	139.123	32.88512

N = number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{\gamma_{1cal}-\gamma_{1\exp}}{\gamma_{1\exp}}\right)+\left(\frac{\gamma_{2cal}-\gamma_{2\exp}}{\gamma_{2\exp}}\right)\right|\right]\text{x}100$$

= ((14.184745+32.88512) x 100)/37

= 127.22%

Table5.37 The liquid and vapor enthalpy of ethanol(1)+water(2) at constant of the enthalpy model =1.01D_1.

No.	x_1	T(K)	Hl_{exp}	Hl_{cal}	$\|(Hl_{cal}-Hl_{exp})/Hl_{exp}\|$	No.	y_1	T(K)	Hv_{exp}	Hv_{cal}	$\|(Hv_{cal}-Hv_{exp})/Hv_{exp}\|$
1	0.2	300	2.25	2.55	0.133333333	1	0.89	351.3	47.5	43.96	0.074526316
2	0.2	330	4.9	5.78	0.179591837	2	0.94	351.4	47.5	48.46	0.020210526
3	0.2	360	7.5	9.36	0.248000000	3	0.79	351.5	47.5	47.92	0.008842105
4	0.4	300	2.5	1.94	0.224000000	4	0.68	352.3	47.5	47.57	0.001473684
5	0.4	330	5.4	4.28	0.207407407	5	0.62	353.5	47.5	47.33	0.003578947
6	0.4	360	8.5	6.80	0.200000000	6	0.58	354.7	47.5	47.14	0.007578947
7	0.6	300	2.7	2.91	0.077777778	7	0.52	356.3	47.6	46.98	0.013025210
8	0.6	330	5.7	6.42	0.126315789	8	0.41	360.3	47.6	46.96	0.013445378
9	0.6	360	8.8	10.2	0.157954545	9	0.33	363.7	47.8	47.01	0.016527197
10	0.8	300	2.7	2.23	0.174074074	10	0.24	366.5	47.8	47.04	0.015899582
11	0.8	330	6.0	4.8	0.200000000	11	0.18	368.3	48.0	47.11	0.018541667
12	0.8	360	9.0	7.44	0.173333333	12	0.10	370.4	48.0	47.04	0.020000000
Sum of data			65.95	64.7	2.101788098	Sum of data			571.8	564.5	0.213649559

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{Hl_{cal}-Hl_{exp}}{Hl_{exp}}\right)+\left(\frac{Hv_{cal}-Hv_{exp}}{Hv_{exp}}\right)\right|\right]x100$$

= ((2.101788098+0.213649559)x100)/12

= 19.30%

Table5.38 The liquid and vapor enthalpy of ethanol(1)+water(2) at constant of the enthalpy model =0.99D_1.

No.	x_1	T(K)	Hl_{exp}	Hl_{cal}	$\lvert(Hl_{cal}-Hl_{exp})/Hl_{exp}\rvert$	No.	y_1	T(K)	Hv_{exp}	Hv_{cal}	$\lvert(Hv_{cal}-Hv_{exp})/Hv_{exp}\rvert$
1	0.2	300	2.25	2.9	0.275555556	1	0.89	351.3	47.5	46.04	0.0307368
2	0.2	330	4.9	6.5	0.316326531	2	0.94	351.4	47.5	50.66	0.0665263
3	0.2	360	7.5	10	0.385333333	3	0.79	351.5	47.5	49.72	0.0467368
4	0.4	300	2.5	2.1	0.160000000	4	0.68	352.3	47.5	49.05	0.0326316
5	0.4	330	5.4	4.6	0.146296296	5	0.62	353.5	47.5	48.55	0.0221053
6	0.4	360	8.5	7.3	0.141176471	6	0.58	354.7	47.5	48.16	0.0138947
7	0.6	300	2.7	3.1	0.162962963	7	0.52	356.3	47.6	47.82	0.0046218
8	0.6	330	5.7	6.9	0.214035088	8	0.41	360.3	47.6	47.55	0.0010504
9	0.6	360	8.8	11.0	0.243181818	9	0.33	363.7	47.8	47.45	0.0073222
10	0.8	300	2.7	2.3	0.148148148	10	0.24	366.5	47.8	47.34	0.0096234
11	0.8	330	6.0	5.0	0.175000000	11	0.18	368.3	48.0	47.32	0.0141667
12	0.8	360	9.0	7.7	0.148888889	12	0.1	370.4	48.0	47.11	0.0185417
Sum of data			65.95	70	2.516905092	Sum of data			571.8	0.268	0.2679578

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{Hl_{cal}-Hl_{exp}}{Hl_{exp}}\right)+\left(\frac{Hv_{cal}-Hv_{exp}}{Hv_{exp}}\right)\right|\right]x100$$

= ((2.516905092+0.2679578)x100)/12

= 23.21%

Table5.39 The liquid and vapor enthalpy of ethanol(1)+water(2) at constant of the enthalpy model =1.02D_1.

No.	x_1	T(K)	Hl_{exp}	Hl_{cal}	$\lvert(Hl_{cal}-Hl_{exp})/Hl_{exp}\rvert$	No.	y_1	T(K)	Hv_{exp}	Hv_{cal}	$\lvert(Hv_{cal}-Hv_{exp})/Hv_{exp}\rvert$
1	0.2	300	2.25	2.39	0.062222222	1	0.89	351.3	47.5	42.92	0.096421053
2	0.2	330	4.9	5.44	0.110204082	2	0.94	351.4	47.5	47.36	0.002947368
3	0.2	360	7.5	8.85	0.180000000	3	0.79	351.5	47.5	47.02	0.010105263
4	0.4	300	2.5	1.86	0.256000000	4	0.68	352.3	47.5	46.83	0.014105263
5	0.4	330	5.4	4.12	0.237037037	5	0.62	353.5	47.5	46.72	0.016421053
6	0.4	360	8.5	6.55	0.229411765	6	0.58	354.7	47.5	46.63	0.018315789
7	0.6	300	2.7	2.79	0.033333333	7	0.52	356.3	47.6	46.57	0.021638655
8	0.6	330	5.7	6.18	0.084210526	8	0.41	360.3	47.6	46.67	0.019537815
9	0.6	360	8.8	9.82	0.115909091	9	0.33	363.7	47.8	46.79	0.021129707
10	0.8	300	2.7	2.2	0.185185185	10	0.24	366.5	47.8	46.9	0.018828452
11	0.8	330	6.0	4.73	0.211666667	11	0.18	368.3	48.0	47.01	0.020625000
12	0.8	360	9.0	7.33	0.185555556	12	0.1	370.4	48.0	47.01	0.020625000
Sum of data			65.95	62.3	1.890735464	Sum of data			571.8	558.4	0.280700419

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{Hl_{cal}-Hl_{exp}}{Hl_{exp}}\right)+\left(\frac{Hv_{cal}-Hv_{exp}}{Hv_{exp}}\right)\right|\right]x100$$

= ((1.890735464+0.280700419)x100)/12

= 18.10%

Table5.40 The liquid and vapor enthalpy of ethanol(1)+water(2) at constant of the enthalpy model =0.98D$_1$.

No.	x_1	T(K)	Hl_{exp}	Hl_{cal}	$\lvert(Hl_{cal}-Hl_{exp})/Hl_{exp}\rvert$	No.	y_1	T(K)	Hv_{exp}	Hv_{cal}	$\lvert(Hv_{cal}-Hv_{exp})/Hv_{exp}\rvert$
1	0.2	300	2.25	3.02	0.342222222	1	0.89	351.3	47.5	47.08	0.008842105
2	0.2	330	4.9	6.78	0.383673469	2	0.94	351.4	47.5	51.75	0.089473684
3	0.2	360	7.5	10.9	0.453333333	3	0.79	351.5	47.5	50.62	0.065684211
4	0.4	300	2.5	2.17	0.132000000	4	0.68	352.3	47.5	49.79	0.048210526
5	0.4	330	5.4	4.77	0.116666667	5	0.62	353.5	47.5	49.16	0.034947368
6	0.4	360	8.5	7.54	0.112941176	6	0.58	354.7	47.5	48.68	0.024842105
7	0.6	300	2.7	3.26	0.207407407	7	0.52	356.3	47.6	48.24	0.013445378
8	0.6	330	5.7	7.16	0.256140351	8	0.41	360.3	47.6	47.86	0.005462185
9	0.6	360	8.8	11.3	0.286363636	9	0.33	363.7	47.8	47.67	0.002719665
10	0.8	300	2.7	2.34	0.133333333	10	0.24	366.5	47.8	47.48	0.006694561
11	0.8	330	6.0	5.02	0.163333333	11	0.18	368.3	48.0	47.43	0.011875.000
12	0.8	360	9.0	7.77	0.136666667	12	0.1	370.4	48.0	47.14	0.017916667
Sum of data			65.95	72.1	2.724081596	Sum of data			571.8	582.9	0.330113456

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{Hl_{cal}-Hl_{exp}}{Hl_{exp}}\right)+\left(\frac{Hv_{cal}-Hv_{exp}}{Hv_{exp}}\right)\right|\right]x100$$

= ((2.724081596+0.330113456)x100)/12

= 25.45%

Table5.41 The liquid and vapor enthalpy of ethanol(1)+water(2) at constant of the enthalpy model =1.03D_1.

No.	x_1	T(K)	Hl_{exp}	Hl_{cal}	$\lvert(Hl_{cal}-Hl_{exp})/Hl_{exp}\rvert$	No.	y_1	T(K)	Hv_{exp}	Hv_{cal}	$\lvert(Hv_{cal}-Hv_{exp})/Hv_{exp}\rvert$
1	0.2	300	2.25	2.23	0.008888889	1	0.89	351.3	47.5	41.88	0.118315789
2	0.2	330	4.9	5.1	0.040816327	2	0.94	351.4	47.5	46.23	0.026736842
3	0.2	360	7.5	8.34	0.112000000	3	0.79	351.5	47.5	46.11	0.029263158
4	0.4	300	2.5	1.78	0.288000000	4	0.68	352.3	47.5	46.09	0.029684211
5	0.4	330	5.4	3.96	0.266666667	5	0.62	353.5	47.5	46.11	0.029263158
6	0.4	360	8.5	6.3	0.258823529	6	0.58	354.7	47.5	46.12	0.029052632
7	0.6	300	2.7	2.68	0.007407407	7	0.52	356.3	47.6	46.15	0.030462185
8	0.6	330	5.7	5.94	0.042105263	8	0.41	360.3	47.6	46.37	0.025840336
9	0.6	360	8.8	9.44	0.072727273	9	0.33	363.7	47.8	46.57	0.025732218
10	0.8	300	2.7	2.17	0.196296296	10	0.24	366.5	47.8	46.75	0.021966527
11	0.8	330	6.0	4.66	0.223333333	11	0.18	368.3	48.0	46.9	0.022916667
12	0.8	360	9.0	7.22	0.197777778	12	0.1	370.4	48.0	46.97	0.021458333
Sum of data			65.95	59.8	1.714842762	Sum of data			571.8	552.3	0.410692055

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{Hl_{cal}-Hl_{exp}}{Hl_{exp}}\right)+\left(\frac{Hv_{cal}-Hv_{exp}}{Hv_{exp}}\right)\right|\right]\text{x}100$$

$$= ((1.714842762+0.410692055)\text{x}100)/12$$

$$= 17.71\%$$

Table5.42 The liquid and vapor enthalpy of ethanol(1)+water(2) at constant of the enthalpy model =0.97D$_1$.

No.	x_1	T(K)	Hl_{exp}	Hl_{cal}	$\lvert(Hl_{cal}-Hl_{exp})/Hl_{exp}\rvert$	No.	y_1	T(K)	Hv_{exp}	Hv_{cal}	$\lvert(Hv_{cal}-Hv_{exp})/Hv_{exp}\rvert$
1	0.2	300	2.25	3.18	0.413333333	1	0.89	351.3	47.5	48.1	0.013052632
2	0.2	330	4.9	7.12	0.453061224	2	0.94	351.4	47.5	52.9	0.112631579
3	0.2	360	7.5	11.4	0.522666667	3	0.79	351.5	47.5	51.5	0.084631579
4	0.4	300	2.5	2.25	0.100000000	4	0.68	352.3	47.5	50.5	0.063789474
5	0.4	330	5.4	4.94	0.085185185	5	0.62	353.5	47.5	49.8	0.047789474
6	0.4	360	8.5	7.79	0.083529412	6	0.58	354.7	47.5	49.2	0.047789474
7	0.6	300	2.7	3.37	0.248148148	7	0.52	356.3	47.6	48.7	0.022268908
8	0.6	330	5.7	7.41	0.300000000	8	0.41	360.3	47.6	48.2	0.011554622
9	0.6	360	8.8	11.7	0.328409091	9	0.33	363.7	47.8	47.9	0.001882845
10	0.8	300	2.7	2.37	0.122222222	10	0.24	366.5	47.8	47.6	0.003556485
11	0.8	330	6.0	5.1	0.150000000	11	0.18	368.3	48.0	47.5	0.009791667
12	0.8	360	9.0	7.89	0.123333333	12	0.1	370.4	48.0	47.2	0.017291667
Sum of data			65.95	74.5	2.929888616	Sum of data			571.8	589	0.436030404

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{Hl_{cal}-Hl_{exp}}{Hl_{exp}}\right)+\left(\frac{Hv_{cal}-Hv_{exp}}{Hv_{exp}}\right)\right|\right]x100$$

$$= ((2.929888616+0.436030404)x100)/12$$

$$= 28.05\%$$

Table5.43 The liquid and vapor enthalpy of ethanol(1)+water(2) at constant of the enthalpy model =1.04D$_1$.

No.	x_1	T(K)	Hl_{exp}	Hl_{cal}	$\lvert(Hl_{cal}-Hl_{exp})/Hl_{exp}\rvert$	No.	y_1	T(K)	Hv_{exp}	Hv_{cal}	$\lvert(Hv_{cal}-Hv_{exp})/Hv_{exp}\rvert$
1	0.2	300	2.25	2.07	0.080000000	1	0.89	351.3	47.5	40.84	0.140210526
2	0.2	330	4.9	4.77	0.026530612	2	0.94	351.4	47.5	45.16	0.049263158
3	0.2	360	7.5	7.83	0.044000000	3	0.79	351.5	47.5	45.21	0.048210526
4	0.4	300	2.5	1.71	0.316000000	4	0.68	352.3	47.5	45.35	0.045263158
5	0.4	330	5.4	3.79	0.298148148	5	0.62	353.5	47.5	45.51	0.041894737
6	0.4	360	8.5	6.05	0.288235294	6	0.58	354.7	47.5	45.61	0.039789474
7	0.6	300	2.7	2.56	0.051851852	7	0.52	356.3	47.6	45.73	0.039285714
8	0.6	330	5.7	5.69	0.001754386	8	0.41	360.3	47.6	46.07	0.032142857
9	0.6	360	8.8	9.07	0.030681818	9	0.33	363.7	47.8	46.36	0.030125523
10	0.8	300	2.7	2.13	0.211111111	10	0.24	366.5	47.8	46.6	0.025104603
11	0.8	330	6.0	4.59	0.235000000	11	0.18	368.3	48.0	46.8	0.025000000
12	0.8	360	9.0	7.11	0.210000000	12	0.1	370.4	48.0	46.94	0.022083333
Sum of data			66	57.4	1.793313222	Sum of data			571.8	546.2	0.538373609

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{Hl_{cal}-Hl_{exp}}{Hl_{exp}}\right)+\left(\frac{Hv_{cal}-Hv_{exp}}{Hv_{exp}}\right)\right|\right]x100$$

= ((1.793313222+0.538373609)x100)/12

= 19.43%

Table5.44 The liquid and vapor enthalpy of ethanol(1)+water(2) at constant of the enthalpy model=0.96D$_1$.

No.	x_1	T(K)	Hl_{exp}	Hl_{cal}	$\lvert(Hl_{cal}-Hl_{exp})/Hl_{exp}\rvert$	No.	y_1	T(K)	Hv_{exp}	Hv_{cal}	$\lvert(Hv_{cal}-Hv_{exp})/Hv_{exp}\rvert$
1	0.2	300	2.25	3.34	0.484444444	1	0.89	351.3	47.5	49.16	0.034947368
2	0.2	330	4.9	7.45	0.520408163	2	0.94	351.4	47.5	53.95	0.135789474
3	0.2	360	7.5	11.93	0.590666667	3	0.79	351.5	47.5	52.42	0.103578947
4	0.4	300	2.5	2.32	0.072000000	4	0.68	352.3	47.5	51.27	0.079368421
5	0.4	330	5.4	5.10	0.055555556	5	0.62	353.5	47.5	50.37	0.060421053
6	0.4	360	8.5	8.04	0.054117647	6	0.58	354.7	47.5	49.7	0.060421053
7	0.6	300	2.7	3.49	0.292592593	7	0.52	356.3	47.6	49.08	0.031092437
8	0.6	330	5.7	7.65	0.342105263	8	0.41	360.3	47.6	48.45	0.017857143
9	0.6	360	8.8	12.07	0.371590909	9	0.33	363.7	47.8	48.1	0.006276151
10	0.8	300	2.7	2.41	0.107407407	10	0.24	366.5	47.8	47.78	0.000418410
11	0.8	330	6.0	5.17	0.138333333	11	0.18	368.3	48.0	47.64	0.007500000
12	0.8	360	9.0	8.0	0.111111111	12	0.10	370.4	48.0	47.2	0.016666667
Sum of data			65.95	76.97	3.140333094	Sum of data			571.8	595.1	0.554337123

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{Hl_{cal}-Hl_{exp}}{Hl_{exp}}\right)+\left(\frac{Hv_{cal}-Hv_{exp}}{Hv_{exp}}\right)\right|\right]x100$$

$$= ((3.140333094+0.554337123)x100)/12$$

$$= 30.79\%$$

Table5.45 The liquid and vapor enthalpy of ethanol(1)+water(2) at constant of the enthalpy model =1.05D$_1$.

No.	x_1	T(K)	Hl_{exp}	Hl_{cal}	$\lvert(Hl_{cal}-Hl_{exp})/Hl_{exp}\rvert$	No.	y_1	T(K)	Hv_{exp}	Hv_{cal}	$\lvert(Hv_{cal}-Hv_{exp})/Hv_{exp}\rvert$
1	0.2	300	2.25	1.91	0.151111111	1	0.89	351.3	47.5	39.8	0.162105263
2	0.2	330	4.9	4.43	0.095918367	2	0.94	351.4	47.5	44.06	0.072421053
3	0.2	360	7.5	7.31	0.025333333	3	0.79	351.5	47.5	44.31	0.067157895
4	0.4	300	2.5	1.63	0.348000000	4	0.68	352.3	47.5	44.61	0.060842105
5	0.4	330	5.4	3.63	0.327777778	5	0.62	353.5	47.5	44.9	0.054736842
6	0.4	360	8.5	5.80	0.317647059	6	0.58	354.7	47.5	45.1	0.050526316
7	0.6	300	2.7	2.44	0.096296296	7	0.52	356.3	47.6	45.31	0.048109244
8	0.6	330	5.7	5.44	0.045614035	8	0.41	360.3	47.6	45.77	0.038445378
9	0.6	360	8.8	8.69	0.012500000	9	0.33	363.7	47.8	46.14	0.034728033
10	0.8	300	2.7	2.1	0.222222222	10	0.24	366.5	47.8	46.46	0.028033473
11	0.8	330	6.0	4.51	0.248333333	11	0.18	368.3	48.0	46.69	0.027291667
12	0.8	360	9.0	6.99	0.223333333	12	0.1	370.4	48.0	46.91	0.022708333
Sum of data			65.95	54.9	2.114086869	Sum of data			571.8	540.1	0.667105602

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{Hl_{cal}-Hl_{exp}}{Hl_{exp}}\right)+\left(\frac{Hv_{cal}-Hv_{exp}}{Hv_{exp}}\right)\right|\right]x100$$

= ((2.114086869+0.667105602)x100)/12

= 23.18%

Table5.46 The liquid and vapor enthalpy of ethanol(1)+water(2) at constant of the enthalpy model =0.95D$_1$.

No.	x_1	T(K)	Hl_{exp}	Hl_{cal}	$\lvert(Hl_{cal}-Hl_{exp})/Hl_{exp}\rvert$	No.	y_1	T(K)	Hv_{exp}	Hv_{cal}	$\lvert(Hv_{cal}-Hv_{exp})/Hv_{exp}\rvert$
1	0.2	300	2.25	3.5	0.555555556	1	0.89	351.3	47.5	50.2	0.056842105
2	0.2	330	4.9	7.79	0.589795918	2	0.94	351.4	47.5	55.05	0.158947368
3	0.2	360	7.5	12.44	0.658666667	3	0.79	351.5	47.5	53.32	0.122526316
4	0.4	300	2.5	2.4	0.040000000	4	0.68	352.3	47.5	52.01	0.094947368
5	0.4	330	5.4	5.26	0.025925926	5	0.62	353.5	47.5	50.98	0.073263158
6	0.4	360	8.5	8.29	0.024705882	6	0.58	354.7	47.5	50.21	0.057052632
7	0.6	300	2.7	3.6	0.333333333	7	0.52	356.3	47.6	49.45	0.038865546
8	0.6	330	5.7	7.9	0.385964912	8	0.41	360.3	47.6	48.75	0.024159664
9	0.6	360	8.8	12.44	0.413636364	9	0.33	363.7	47.8	48.32	0.010878661
10	0.8	300	2.7	2.44	0.096296296	10	0.24	366.5	47.8	47.92	0.00251046
11	0.8	330	6.0	5.24	0.126666667	11	0.18	368.3	48.0	47.74	0.005416667
12	0.8	360	9.0	8.11	0.098888889	12	0.1	370.4	48.0	47.24	0.015833333
Sum of data			65.95	79.41	3.34943641	Sum of data			571.8	601.2	0.661243279

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{Hl_{cal}-Hl_{exp}}{Hl_{exp}}\right)+\left(\frac{Hv_{cal}-Hv_{exp}}{Hv_{exp}}\right)\right|\right]x100$$

= ((3.34943641+0.661243279)x100)/12

= 33.42%

Table5.47 The liquid and vapor enthalpy of ethanol(1)+water(2) at constant of the enthalpy model =1.06D_1.

No.	x_1	T(K)	Hl_{exp}	Hl_{cal}	$\|(Hl_{cal}-Hl_{exp})/Hl_{exp}\|$	No.	y_1	T(K)	Hv_{exp}	Hv_{cal}	$\|(Hv_{cal}-Hv_{exp})/Hv_{exp}\|$
1	0.2	300	2.25	1.76	0.217777778	1	0.89	351.3	47.5	38.76	0.184000000
2	0.2	330	4.9	4.1	0.163265306	2	0.94	351.4	47.5	42.96	0.095578947
3	0.2	360	7.5	6.8	0.093333333	3	0.79	351.5	47.5	43.41	0.086105263
4	0.4	300	2.5	1.55	0.380000000	4	0.68	352.3	47.5	43.87	0.076421053
5	0.4	330	5.4	3.47	0.357407407	5	0.62	353.5	47.5	44.29	0.067578947
6	0.4	360	8.5	5.55	0.347058824	6	0.58	354.7	47.5	44.89	0.054947368
7	0.6	300	2.7	2.33	0.137037037	7	0.52	356.3	47.6	45.47	0.044747899
8	0.6	330	5.7	5.2	0.087719298	8	0.41	360.3	47.6	45.92	0.035294118
9	0.6	360	8.8	8.32	0.054545455	9	0.33	363.7	47.8	46.31	0.031171548
10	0.8	300	2.7	2.06	0.237037037	10	0.24	366.5	47.8	46.59	0.025313808
11	0.8	330	6.0	4.44	0.260000000	11	0.18	368.3	48.0	46.59	0.029375000
12	0.8	360	9.0	6.88	0.235555556	12	0.1	370.4	48.0	46.88	0.023333333
Sum of data			65.95	52.46	2.570737031	Sum of data			571.8	535.9	0.753867285

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{Hl_{cal}-Hl_{exp}}{Hl_{exp}}\right)+\left(\frac{Hv_{cal}-Hv_{exp}}{Hv_{exp}}\right)\right|\right]x100$$

= ((2.570737031+0.753867285)x100)/12

= 27.72%

Table5.48 The liquid and vapor enthalpy of ethanol(1)+water(2) at constant of the enthalpy model =0.40D$_1$.

No.	x_1	T(K)	Hl_{exp}	Hl_{cal}	$\lvert(Hl_{cal}-Hl_{exp})/Hl_{exp}\rvert$	No.	y_1	T(K)	Hv_{exp}	Hv_{cal}	$\lvert(Hv_{cal}-Hv_{exp})/Hv_{exp}\rvert$
1	0.2	300	2.25	3.66	0.626666667	1	0.89	351.3	47.5	51.24	0.078736842
2	0.2	330	4.9	8.13	0.659183673	2	0.94	351.4	47.5	56.16	0.182315789
3	0.2	360	7.5	12.95	0.726666667	3	0.79	351.5	47.5	54.23	0.141684211
4	0.4	300	2.5	2.48	0.008000000	4	0.68	352.3	47.5	52.75	0.110526316
5	0.4	330	5.4	5.43	0.005555556	5	0.62	353.5	47.5	51.59	0.086105263
6	0.4	360	8.5	8.54	0.004705882	6	0.58	354.7	47.5	50.72	0.067789474
7	0.6	300	2.7	3.72	0.377777778	7	0.52	356.3	47.6	49.91	0.048529412
8	0.6	330	5.7	8.14	0.428070175	8	0.41	360.3	47.6	49.05	0.030462185
9	0.6	360	8.8	12.82	0.456818182	9	0.33	363.7	47.8	48.54	0.015481172
10	0.8	300	2.7	2.48	0.081481481	10	0.24	366.5	47.8	48.07	0.005648536
11	0.8	330	6.0	5.32	0.113333333	11	0.18	368.3	48.0	47.85	0.003125000
12	0.8	360	9.0	8.22	0.086666667	12	0.1	370.4	48.0	47.27	0.015208333
Sum of data			65.95	81.89	3.574926061	Sum of data			571.8	607.4	0.785612532

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{Hl_{cal}-Hl_{exp}}{Hl_{exp}}\right)+\left(\frac{Hv_{cal}-Hv_{exp}}{Hv_{exp}}\right)\right|\right]x100$$

= ((3.574926061+0.785612532)x100)/12

= 36.34%

Table5.49 The liquid and vapor enthalpy of ethanol(1)+water(2) at constant of the enthalpy model =1.07D_1.

No.	x_1	T(K)	Hl_{exp}	Hl_{cal}	$\lvert(Hl_{cal}-Hl_{exp})/Hl_{exp}\rvert$	No.	y_1	T(K)	Hv_{exp}	Hv_{cal}	$\lvert(Hv_{cal}-Hv_{exp})/Hv_{exp}\rvert$
1	0.2	300	2.25	1.6	0.288888889	1	0.89	351.3	47.5	37.72	0.205894737
2	0.2	330	4.9	3.76	0.232653061	2	0.94	351.4	47.5	41.86	0.118736842
3	0.2	360	7.5	6.29	0.161333333	3	0.79	351.5	47.5	42.51	0.105052632
4	0.4	300	2.5	1.48	0.408000000	4	0.68	352.3	47.5	43.13	0.092000000
5	0.4	330	5.4	3.3	0.388888889	5	0.62	353.5	47.5	43.68	0.080421053
6	0.4	360	8.5	5.3	0.376470588	6	0.58	354.7	47.5	44.08	0.072000000
7	0.6	300	2.7	2.21	0.181481481	7	0.52	356.3	47.6	44.47	0.065756303
8	0.6	330	5.7	4.95	0.131578947	8	0.41	360.3	47.6	45.18	0.050840336
9	0.6	360	8.8	7.94	0.097727273	9	0.33	363.7	47.8	45.7	0.043933054
10	0.8	300	2.7	2.03	0.248148148	10	0.24	366.5	47.8	46.17	0.034100418
11	0.8	330	6.0	4.37	0.271666667	11	0.18	368.3	48.0	46.48	0.031666667
12	0.8	360	9.0	6.77	0.247777778	12	0.1	370.4	48.0	46.84	0.024166667
Sum of data			65.95	50	3.034615055	Sum of data			571.8	527.8	0.924568708

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{Hl_{cal}-Hl_{exp}}{Hl_{exp}}\right)+\left(\frac{Hv_{cal}-Hv_{exp}}{Hv_{exp}}\right)\right|\right]x100$$

= ((3.034615055+0.924568708)x100)/12

= 32.99%

Table5.50 The liquid and vapor enthalpy of ethanol(1)+water(2) at constant of the enthalpy model =0.93D_1.

No.	x_1	T(K)	Hl_{exp}	Hl_{cal}	$\lvert(Hl_{cal}-Hl_{exp})/Hl_{exp}\rvert$	No.	y_1	T(K)	Hv_{exp}	Hv_{cal}	$\lvert(Hv_{cal}-Hv_{exp})/Hv_{exp}\rvert$
1	0.2	300	2.25	3.82	0.697777778	1	0.89	351.3	47.5	52.28	0.100631579
2	0.2	330	4.9	8.46	0.726530612	2	0.94	351.4	47.5	57.25	0.205263158
3	0.2	360	7.5	13.47	0.796000000	3	0.79	351.5	47.5	55.13	0.160631579
4	0.4	300	2.5	2.56	0.024000000	4	0.68	352.3	47.5	53.49	0.126105263
5	0.4	330	5.4	5.59	0.035185185	5	0.62	353.5	47.5	52.2	0.098947368
6	0.4	360	8.5	8.79	0.034117647	6	0.58	354.7	47.5	51.23	0.078526316
7	0.6	300	2.7	3.83	0.418518519	7	0.52	356.3	47.6	50.33	0.057352941
8	0.6	330	5.7	8.39	0.471929825	8	0.41	360.3	47.6	49.34	0.036554622
9	0.6	360	8.8	13.19	0.498863636	9	0.33	363.7	47.8	48.76	0.020083682
10	0.8	300	2.7	2.51	0.07037037	10	0.24	366.5	47.8	48.22	0.008786611
11	0.8	330	6.0	5.39	0.101666667	11	0.18	368.3	48.0	47.95	0.001041667
12	0.8	360	9.0	8.33	0.074444444	12	0.1	370.4	48.0	47.3	0.014583333
Sum of data			65.95	84.33	3.949404683	Sum of data			571.8	613.5	0.908508119

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{Hl_{cal}-Hl_{exp}}{Hl_{exp}}\right)+\left(\frac{Hv_{cal}-Hv_{exp}}{Hv_{exp}}\right)\right|\right]x100$$

= ((3.949404683+0.908508119)x100)/12

= 40.48%

Table5.51 The liquid and vapor enthalpy of ethanol(1)+water(2) at constant of the enthalpy model =1.08D_1.

No.	x_1	T(K)	Hl_{exp}	Hl_{cal}	$\lvert(Hl_{cal}-Hl_{exp})/Hl_{exp}\rvert$	No.	y_1	T(K)	Hv_{exp}	Hv_{cal}	$\lvert(Hv_{cal}-Hv_{exp})/Hv_{exp}\rvert$
1	0.2	300	2.25	1.44	0.360000000	1	0.89	351.3	47.5	36.68	0.227789474
2	0.2	330	4.9	3.43	0.300000000	2	0.94	351.4	47.5	40.76	0.141894737
3	0.2	360	7.5	5.77	0.230666667	3	0.79	351.5	47.5	41.61	0.124000000
4	0.4	300	2.5	1.39	0.444000000	4	0.68	352.3	47.5	42.39	0.107578947
5	0.4	330	5.4	3.14	0.418518519	5	0.62	353.5	47.5	43.07	0.093263158
6	0.4	360	8.5	5.05	0.405882353	6	0.58	354.7	47.5	43.57	0.082736842
7	0.6	300	2.7	2.1	0.222222222	7	0.52	356.3	47.6	44.05	0.074579832
8	0.6	330	5.7	4.7	0.175438596	8	0.41	360.3	47.6	44.88	0.057142857
9	0.6	360	8.8	7.57	0.139772727	9	0.33	363.7	47.8	45.48	0.048535565
10	0.8	300	2.7	1.99	0.262962963	10	0.24	366.5	47.8	46.02	0.037238494
11	0.8	330	6.0	4.29	0.285000000	11	0.18	368.3	48.0	46.37	0.033958333
12	0.8	360	9.0	6.66	0.260000000	12	0.1	370.4	48.0	46.81	0.024791667
Sum of data			65.95	47.53	3.504464047	Sum of data			571.8	521.7	1.053509906

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{Hl_{cal}-Hl_{exp}}{Hl_{exp}}\right)+\left(\frac{Hv_{cal}-Hv_{exp}}{Hv_{exp}}\right)\right|\right]x100$$

= ((3.504464047+1.053509906)x100)/12

= 37.98%

Table5.52 The liquid and vapor enthalpy of ethanol(1)+water(2) at constant of the enthalpy model =0.92D$_1$.

No.	x_1	T(K)	Hl_{exp}	Hl_{cal}	$\lvert(Hl_{cal}-Hl_{exp})/Hl_{exp}\rvert$	No.	y_1	T(K)	Hv_{exp}	Hv_{cal}	$\lvert(Hv_{cal}-Hv_{exp})/Hv_{exp}\rvert$
1	0.2	300	2.25	3.98	0.768888889	1	0.89	351.3	47.5	53.31	0.122315789
2	0.2	330	4.9	8.80	0.795918367	2	0.94	351.4	47.5	58.35	0.228421053
3	0.2	360	7.5	13.98	0.864000000	3	0.79	351.5	47.5	56.03	0.179578947
4	0.4	300	2.5	2.63	0.052000000	4	0.68	352.3	47.5	54.23	0.141684211
5	0.4	330	5.4	5.75	0.064814815	5	0.62	353.5	47.5	52.81	0.111789474
6	0.4	360	8.5	9.04	0.063529412	6	0.58	354.7	47.5	51.74	0.089263158
7	0.6	300	2.7	3.95	0.462962963	7	0.52	356.3	47.6	50.75	0.066176471
8	0.6	330	5.7	8.63	0.514035088	8	0.41	360.3	47.6	49.64	0.042857143
9	0.6	360	8.8	13.57	0.542045455	9	0.33	363.7	47.8	48.98	0.024686192
10	0.8	300	2.7	2.55	0.055555556	10	0.24	366.5	47.8	48.36	0.011715481
11	0.8	330	6.0	5.46	0.090000000	11	0.18	368.3	48.0	48.06	0.001250000
12	0.8	360	9.0	8.44	0.062222222	12	0.1	370.4	48.0	47.33	0.013958333
Sum of data			65.95	86.78	4.335972766	Sum of data			571.8	619.6	1.033696252

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{Hl_{cal}-Hl_{exp}}{Hl_{exp}}\right)+\left(\frac{Hv_{cal}-Hv_{exp}}{Hv_{exp}}\right)\right|\right]x100$$

= ((4.335972766+1.033696252)x100)/12

= 44.75%

Table5.53 The liquid and vapor enthalpy of ethanol(1)+water(2) at constant of the enthalpy model =1.09D$_1$.

No.	x_1	T(K)	Hl_{exp}	Hl_{cal}	$\lvert(Hl_{cal}-Hl_{exp})/Hl_{exp}\rvert$	No.	y_1	T(K)	Hv_{exp}	Hv_{cal}	$\lvert(Hv_{cal}-Hv_{exp})/Hv_{exp}\rvert$
1	0.2	300	2.25	1.28	0.431111111	1	0.89	351.3	47.5	35.64	0.249684211
2	0.2	330	4.9	3.09	0.369387755	2	0.94	351.4	47.5	39.67	0.164842105
3	0.2	360	7.5	5.26	0.298666667	3	0.79	351.5	47.5	40.71	0.142947368
4	0.4	300	2.5	1.32	0.472000000	4	0.68	352.3	47.5	41.65	0.123157895
5	0.4	330	5.4	2.98	0.448148148	5	0.62	353.5	47.5	42.46	0.106105263
6	0.4	360	8.5	4.8	0.435294118	6	0.58	354.7	47.5	43.05	0.093684211
7	0.6	300	2.7	1.98	0.266666667	7	0.52	356.3	47.6	43.64	0.083193277
8	0.6	330	5.7	4.46	0.217543860	8	0.41	360.3	47.6	44.58	0.063445378
9	0.6	360	8.8	7.2	0.181818182	9	0.33	363.7	47.8	45.26	0.053138075
10	0.8	300	2.7	1.96	0.274074074	10	0.24	366.5	47.8	45.87	0.040376569
11	0.8	330	6.0	4.22	0.296666667	11	0.18	368.3	48.0	46.27	0.036041667
12	0.8	360	9.0	6.55	0.272222222	12	0.1	370.4	48.0	46.78	0.025416667
Sum of data			65.95	45.1	3.96359947	Sum of data			571.8	515.6	1.182032686

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{Hl_{cal}-Hl_{exp}}{Hl_{exp}}\right)+\left(\frac{Hv_{cal}-Hv_{exp}}{Hv_{exp}}\right)\right|\right]x100$$

= ((3.96359947+1.182032686)x100)/12

= 42.88%

Table5.54 The liquid and vapor enthalpy of ethanol(1)+water(2) at constant of the enthalpy model =0.91D_1.

No.	x_1	T(K)	Hl_{exp}	Hl_{cal}	$\|(Hl_{cal}-Hl_{exp})/Hl_{exp}\|$	No.	y_1	T(K)	Hv_{exp}	Hv_{cal}	$\|(Hv_{cal}-Hv_{exp})/Hv_{exp}\|$
1	0.2	300	2.25	4.13	0.835555556	1	0.89	351.3	47.5	54.35	0.144210526
2	0.2	330	4.9	9.13	0.863265306	2	0.94	351.4	47.5	59.45	0.251578947
3	0.2	360	7.5	14.49	0.932000000	3	0.79	351.5	47.5	56.93	0.198526316
4	0.4	300	2.5	2.71	0.084000000	4	0.68	352.3	47.5	54.97	0.157263158
5	0.4	330	5.4	5.92	0.096296296	5	0.62	353.5	47.5	53.42	0.124631579
6	0.4	360	8.5	9.29	0.092941176	6	0.58	354.7	47.5	52.25	0.100000000
7	0.6	300	2.7	4.07	0.507407407	7	0.52	356.3	47.6	51.17	0.075000000
8	0.6	330	5.7	8.88	0.557894737	8	0.41	360.3	47.6	49.94	0.049159664
9	0.6	360	8.8	13.94	0.584090909	9	0.33	363.7	47.8	49.2	0.029288703
10	0.8	300	2.7	2.58	0.044444444	10	0.24	366.5	47.8	48.51	0.014853556
11	0.8	330	6.0	5.53	0.078333333	11	0.18	368.3	48.0	48.16	0.003333333
12	0.8	360	9.0	8.56	0.048888889	12	0.1	370.4	48.0	47.37	0.013125000
Sum of data			65.95	89.23	4.725118054	Sum of data			571.8	625.7	1.160970783

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{Hl_{cal}-Hl_{exp}}{Hl_{exp}}\right)+\left(\frac{Hv_{cal}-Hv_{exp}}{Hv_{exp}}\right)\right|\right]x100$$

= ((4.725118054+1.160970783)x100)/12

= 49.05%

Table5.55 The liquid and vapor enthalpy of ethanol(1)+water(2) at constant of the enthalpy model =1.10D_1.

No.	x_1	T(K)	Hl_{exp}	Hl_{cal}	$\lvert(Hl_{cal}-Hl_{exp})/Hl_{exp}\rvert$	No.	y_1	T(K)	Hv_{exp}	Hv_{cal}	$\lvert(Hv_{cal}-Hv_{exp})/Hv_{exp}\rvert$
1	0.2	300	2.25	1.12	0.502222222	1	0.89	351.3	47.5	34.61	0.271368421
2	0.2	330	4.9	2.75	0.438775510	2	0.94	351.4	47.5	38.57	0.188000000
3	0.2	360	7.5	4.75	0.366666667	3	0.79	351.5	47.5	39.81	0.161894737
4	0.4	300	2.5	1.24	0.504000000	4	0.68	352.3	47.5	40.91	0.138736842
5	0.4	330	5.4	2.81	0.479629630	5	0.62	353.5	47.5	41.85	0.118947368
6	0.4	360	8.5	4.55	0.464705882	6	0.58	354.7	47.5	42.54	0.104421053
7	0.6	300	2.7	1.87	0.307407407	7	0.52	356.3	47.6	43.22	0.092016807
8	0.6	330	5.7	4.22	0.259649123	8	0.41	360.3	47.6	44.28	0.069747899
9	0.6	360	8.8	6.82	0.225000000	9	0.33	363.7	47.8	45.04	0.057740586
10	0.8	300	2.7	1.92	0.288888889	10	0.24	366.5	47.8	45.73	0.043305439
11	0.8	330	6.0	4.15	0.308333333	11	0.18	368.3	48.0	46.16	0.038333333
12	0.8	360	9.0	6.44	0.284444444	12	0.1	370.4	48.0	46.75	0.026041667
Sum of data			65.95	42.64	4.429723108	Sum of data			571.8	509.5	1.310554152

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{Hl_{cal}-Hl_{exp}}{Hl_{exp}}\right)+\left(\frac{Hv_{cal}-Hv_{exp}}{Hv_{exp}}\right)\right|\right]x100$$

= ((4.429723108+1.310554152)x100)/12

= 47.83%

Table5.56 The liquid and vapor enthalpy of ethanol(1)+water(2) at constant of the enthalpy model =0.90D$_1$.

No.	x_1	T(K)	Hl_{exp}	Hl_{cal}	$\lvert(Hl_{cal}-Hl_{exp})/Hl_{exp}\rvert$	No.	y_1	T(K)	Hv_{exp}	Hv_{cal}	$\lvert(Hv_{cal}-Hv_{exp})/Hv_{exp}\rvert$
1	0.2	300	2.25	4.29	0.906666667	1	0.89	351.3	47.5	55.39	0.166105263
2	0.2	330	4.9	9.47	0.932653061	2	0.94	351.4	47.5	60.55	0.274736842
3	0.2	360	7.5	15.01	1.001333333	3	0.79	351.5	47.5	57.83	0.217473684
4	0.4	300	2.5	2.79	0.116000000	4	0.68	352.3	47.5	55.71	0.172842105
5	0.4	330	5.4	6.08	0.125925926	5	0.62	353.5	47.5	54.03	0.137473684
6	0.4	360	8.5	9.54	0.122352941	6	0.58	354.7	47.5	52.76	0.110736842
7	0.6	300	2.7	4.18	0.548148148	7	0.52	356.3	47.6	51.59	0.083823529
8	0.6	330	5.7	9.12	0.600000000	8	0.41	360.3	47.6	50.24	0.055462185
9	0.6	360	8.8	14.31	0.626136364	9	0.33	363.7	47.8	49.42	0.033891213
10	0.8	300	2.7	2.61	0.033333333	10	0.24	366.5	47.8	48.65	0.017782427
11	0.8	330	6.0	5.61	0.065000000	11	0.18	368.3	48.0	48.27	0.005625000
12	0.8	360	9.0	8.67	0.036666667	12	0.1	370.4	48.0	47.4	0.01250000
Sum of data			65.95	91.68	5.11421644	Sum of data			571.8	631.8	1.288452776

N= number of data points

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\left(\frac{Hl_{cal}-Hl_{exp}}{Hl_{exp}}\right)+\left(\frac{Hv_{cal}-Hv_{exp}}{Hv_{exp}}\right)\right|\right]x100$$

= ((5.11421644+1.288452776)x100)/12

= 53.36%

Table5.58 Data of liquid composition and temperature profile with accurate property models from computational program and experiment.

Plate	Mole fraction (x_{1cal})	Mole fraction (x_{1exp})	Temperature T_{cal} (K)	Temperature T_{exp} (K)
1	0.755	0.755	351.921	352.55
2	0.725	0.736	352.028	352.75
3	0.696	0.715	352.147	353.25
4	0.667	0.690	352.282	353.55
5	0.637	0.662	352.439	353.25
6	0.602	0.620	352.634	353.45
7	0.560	0.591	352.898	353.75
8	0.502	0.540	353.304	354.35
9	0.413	0.462	354.027	355.3
10	0.274	0.283	355.505	356.05
11	0.268	0.264	355.582	357.15
12	0.231	0.263	356.11	357.15

Table5.59 Simulation results using accuracy property models.

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.994	0.006	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.989	0.011	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.980	0.020	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.963	0.037	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.932	0.068	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.879	0.121	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.793	0.207	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.670	0.330	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.519	0.481	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.363	0.637	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.234	0.766	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.786	0.214	0.801	0.199	0.000	64.742	351.827	48.929	8.757
2	0.755	0.245	0.781	0.219	102.252	64.831	351.921	48.833	8.683
3	0.725	0.275	0.764	0.236	102.341	64.912	352.028	48.752	8.617
4	0.696	0.304	0.749	0.251	102.422	64.992	352.147	48.678	8.555
5	0.667	0.333	0.735	0.265	102.502	65.078	352.282	48.608	8.495
6	0.637	0.363	0.720	0.280	102.588	65.183	352.439	48.536	8.431
7	0.602	0.398	0.704	0.296	102.693	65.325	352.634	48.454	8.355
8	0.560	0.440	0.683	0.317	102.835	65.537	352.898	48.351	8.256
9	0.502	0.498	0.656	0.344	103.047	65.875	353.304	48.206	8.110
10	0.413	0.587	0.615	0.385	103.385	66.393	354.027	47.982	7.872
11	0.274	0.726	0.553	0.447	103.903	263.15	355.505	47.631	7.475
12	0.268	0.732	0.552	0.448	104.36	263.333	355.582	47.622	7.465
13	0.231	0.768	0.533	0.467	104.543	263.445	356.11	47.526	7.355
14	0.101	0.899	0.431	0.569	104.655	158.800	359.443	47.205	7.016

Table5.60 Simulation results using %AAD of the K-value = +6.66%. (1.10A_{21})

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.993	0.006	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.988	0.012	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.979	0.021	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.961	0.039	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.930	0.070	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.876	0.124	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.790	0.210	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.667	0.333	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.516	0.484	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.362	0.638	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.234	0.766	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.804	0.196	0.833	0.166	0.000	64.742	352.11	49.136	8.889
2	0.775	0.225	0.812	0.188	102.252	64.855	352.221	49.039	8.816
3	0.747	0.253	0.792	0.208	102.365	64.973	352.339	48.949	8.746
4	0.720	0.280	0.772	0.228	102.483	65.103	352.47	48.858	8.674
5	0.690	0.310	0.751	0.249	102.613	65.253	352.623	48.762	8.594
6	0.656	0.344	0.727	0.273	102.763	65.426	352.817	48.652	8.499
7	0.614	0.386	0.700	0.300	102.936	65.627	353.079	48.524	8.383
8	0.560	0.440	0.668	0.332	103.137	65.860	353.454	48.373	8.239
9	0.488	0.512	0.632	0.368	103.37	66.139	354.017	48.191	8.055
10	0.392	0.608	0.589	0.411	103.649	66.497	354.893	47.966	7.817
11	0.270	0.730	0.534	0.466	104.007	263.571	356.326	47.676	7.499
12	0.259	0.741	0.527	0.473	104.781	263.623	356.488	47.641	7.461
13	0.211	0.789	0.501	0.499	104.833	263.543	357.253	47.523	7.333
14	0.088	0.912	0.392	0.608	104.753	158.800	360.864	47.233	7.062

Table5.61 Simulation results using %AAD of the K-value = -6.30%. (0.90A_{21})

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.994	0.006	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.989	0.011	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.981	0.019	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.964	0.036	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.934	0.066	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.882	0.118	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.798	0.202	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.675	0.325	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.522	0.478	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.365	0.635	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.233	0.767	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.234	0.766	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.794	0.206	0.799	0.201	0.000	64.742	351.415	48.864	8.734
2	0.776	0.224	0.782	0.218	102.252	64.854	351.449	48.777	8.668
3	0.756	0.244	0.765	0.235	102.364	64.961	351.496	48.69	8.599
4	0.732	0.268	0.748	0.252	102.471	65.064	351.559	48.605	8.527
5	0.705	0.295	0.732	0.268	102.574	65.164	351.645	48.52	8.454
6	0.674	0.326	0.716	0.284	102.674	65.271	351.763	48.434	8.376
7	0.637	0.363	0.699	0.301	102.781	65.399	351.924	48.343	8.291
8	0.591	0.409	0.680	0.320	102.909	65.580	352.155	48.239	8.188
9	0.529	0.471	0.657	0.343	103.090	65.890	352.515	48.104	8.048
10	0.435	0.565	0.622	0.378	103.400	66.465	353.172	47.894	7.817
11	0.278	0.722	0.563	0.437	103.975	262.762	354.663	47.527	7.387
12	0.268	0.732	0.560	0.440	103.972	262.829	354.788	47.507	7.363
13	0.226	0.774	0.544	0.456	104.039	262.897	355.354	47.421	7.261
14	0.094	0.906	0.448	0.552	104.107	158.800	358.888	47.136	6.942

Table5.62 Simulation results using %AAD of the K-value = +9.25%. (1.15A_{21})

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.993	0.007	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.988	0.012	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.979	0.021	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.961	0.039	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.930	0.070	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.875	0.124	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.789	0.211	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.666	0.334	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.516	0.484	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.362	0.638	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.234	0.766	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.807	0.193	0.838	0.162	0.000	64.742	352.255	49.179	8.910
2	0.773	0.227	0.813	0.187	102.252	64.863	352.403	49.07	8.828
3	0.741	0.259	0.790	0.210	102.373	64.986	352.557	48.97	8.750
4	0.709	0.291	0.768	0.232	102.496	65.118	352.724	48.873	8.671
5	0.676	0.324	0.745	0.255	102.628	65.266	352.915	48.771	8.586
6	0.639	0.361	0.720	0.280	102.776	65.436	353.149	48.659	8.488
7	0.595	0.405	0.692	0.308	102.946	65.632	353.454	48.531	8.372
8	0.539	0.461	0.660	0.340	103.142	65.859	353.873	48.38	8.228
9	0.468	0.532	0.624	0.376	103.369	66.126	354.476	48.201	8.048
10	0.377	0.623	0.581	0.419	103.636	66.452	355.372	47.983	7.819
11	0.266	0.734	0.527	0.473	103.962	263.706	356.752	47.712	7.528
12	0.254	0.746	0.520	0.480	104.916	263.769	356.923	47.677	7.490
13	0.208	0.792	0.493	0.507	104.979	263.715	357.704	47.558	7.363
14	0.089	0.911	0.384	0.616	104.925	158.8	361.239	47.261	7.095

Table5.63 Simulation results using %AAD of the K-value = -9.99%. (0.85A_{21})

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.994	0.006	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.990	0.010	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.981	0.019	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.965	0.035	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.936	0.064	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.884	0.116	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.800	0.200	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.678	0.322	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.524	0.476	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.366	0.634	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.233	0.767	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.234	0.766	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.785	0.215	0.798	0.202	0.000	64.742	351.205	48.827	8.720
2	0.777	0.223	0.788	0.212	102.252	64.842	351.220	48.775	8.681
3	0.765	0.235	0.776	0.224	102.352	64.953	351.242	48.711	8.632
4	0.749	0.251	0.761	0.239	102.463	65.070	351.275	48.637	8.571
5	0.729	0.271	0.746	0.254	102.580	65.192	351.325	48.553	8.501
6	0.702	0.298	0.729	0.271	102.702	65.321	351.402	48.461	8.421
7	0.668	0.332	0.710	0.29	102.831	65.468	351.521	48.359	8.327
8	0.622	0.378	0.690	0.310	102.978	65.662	351.711	48.243	8.215
9	0.559	0.441	0.665	0.335	103.172	65.981	352.032	48.096	8.063
10	0.459	0.541	0.630	0.370	103.491	66.592	352.652	47.877	7.821
11	0.286	0.714	0.570	0.430	104.102	262.716	354.152	47.488	7.359
12	0.277	0.723	0.566	0.434	103.926	262.763	354.256	47.462	7.328
13	0.233	0.767	0.549	0.451	103.973	262.706	354.824	47.366	7.212
14	0.093	0.907	0.450	0.550	103.916	158.800	358.488	47.093	6.899

Table5.64 Simulation results using %AAD of the K-value = +22.77%. (1.45A_{21})

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.993	0.006	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.988	0.012	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.979	0.021	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.961	0.039	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.93	0.07	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.876	0.124	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.790	0.210	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.667	0.333	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.516	0.484	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.362	0.638	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.234	0.766	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.812	0.188	0.854	0.146	0.000	64.742	353.009	49.371	8.997
2	0.748	0.252	0.808	0.192	102.252	64.919	353.487	49.203	8.863
3	0.688	0.312	0.766	0.234	102.429	65.086	353.968	49.048	8.736
4	0.63	0.37	0.727	0.273	102.596	65.246	354.467	48.902	8.611
5	0.574	0.426	0.691	0.309	102.756	65.395	354.995	48.76	8.487
6	0.517	0.482	0.657	0.343	102.905	65.535	355.559	48.623	8.363
7	0.462	0.538	0.624	0.376	103.045	65.669	356.162	48.49	8.241
8	0.407	0.593	0.594	0.406	103.179	65.81	356.805	48.36	8.119
9	0.353	0.647	0.563	0.437	103.32	65.978	357.493	48.228	7.994
10	0.300	0.700	0.530	0.470	103.488	66.194	358.256	48.083	7.855
11	0.245	0.755	0.490	0.510	103.704	264.446	359.161	47.911	7.692
12	0.233	0.767	0.483	0.517	105.656	264.598	359.371	47.882	7.665
13	0.193	0.807	0.452	0.548	105.808	264.704	360.171	47.756	7.549
14	0.094	0.906	0.348	0.652	105.914	158.800	363.108	47.426	7.287

Table5.65 Simulation results using %AAD of the K-value = -22.20%. (0.70A_{21})

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.995	0.005	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.991	0.009	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.984	0.016	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.969	0.031	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.942	0.058	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.893	0.107	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.812	0.188	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.690	0.310	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.534	0.466	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.371	0.629	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.233	0.767	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.233	0.767	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.235	0.765	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.724	0.276	0.748	0.252	0.000	64.742	350.517	48.441	8.465
2	0.715	0.285	0.752	0.248	102.252	64.712	350.526	48.464	8.485
3	0.712	0.288	0.756	0.244	102.222	64.711	350.527	48.488	8.505
4	0.712	0.288	0.758	0.242	102.221	64.746	350.526	48.501	8.515
5	0.711	0.289	0.757	0.243	102.256	64.820	350.528	48.494	8.510
6	0.706	0.294	0.751	0.249	102.330	64.940	350.541	48.462	8.483
7	0.692	0.308	0.740	0.260	102.450	65.114	350.572	48.398	8.428
8	0.666	0.334	0.723	0.277	102.624	65.364	350.643	48.295	8.336
9	0.617	0.383	0.698	0.302	102.874	65.768	350.807	48.14	8.186
10	0.519	0.481	0.661	0.339	103.278	66.607	351.239	47.889	7.915
11	0.303	0.697	0.598	0.402	104.117	262.213	352.691	47.395	7.315
12	0.304	0.696	0.598	0.402	103.423	262.446	352.681	47.397	7.316
13	0.274	0.726	0.586	0.414	103.656	262.555	352.978	47.311	7.207
14	0.113	0.887	0.493	0.507	103.765	158.800	356.173	46.992	6.797

Table5.66 Simulation results using %AAD of the K-value = +31.74%. (1.70A_{21})

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.994	0.006	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.989	0.011	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.980	0.02	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.964	0.036	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.933	0.067	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.881	0.119	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.796	0.204	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.673	0.327	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.520	0.480	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.364	0.636	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.233	0.767	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.797	0.203	0.859	0.141	0.000	64.742	353.643	49.483	9.040
2	0.707	0.293	0.796	0.204	102.252	64.951	354.541	49.287	8.875
3	0.625	0.375	0.738	0.262	102.461	65.148	355.414	49.101	8.717
4	0.551	0.449	0.687	0.313	102.658	65.329	356.262	48.923	8.566
5	0.484	0.516	0.640	0.360	102.839	65.489	357.082	48.756	8.422
6	0.424	0.576	0.599	0.401	102.999	65.627	357.863	48.602	8.289
7	0.373	0.627	0.563	0.437	103.137	65.745	358.593	48.464	8.168
8	0.329	0.671	0.533	0.467	103.255	65.851	359.261	48.341	8.062
9	0.292	0.708	0.506	0.494	103.361	65.954	359.861	48.232	7.968
10	0.261	0.739	0.481	0.519	103.464	66.065	360.404	48.132	7.882
11	0.234	0.766	0.457	0.543	103.575	265.018	360.906	48.035	7.800
12	0.220	0.78	0.446	0.554	106.228	265.136	361.183	47.991	7.763
13	0.181	0.819	0.411	0.589	106.346	265.277	362.032	47.855	7.652
14	0.097	0.903	0.313	0.687	106.487	158.800	364.562	47.525	7.419

Table5.67 Simulation results using %AAD of the K-value = -32.04%. (0.60A_{21})

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.996	0.004	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.992	0.008	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.986	0.014	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.973	0.027	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.947	0.053	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.901	0.099	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.822	0.178	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.701	0.299	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.542	0.458	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.375	0.625	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.233	0.767	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.233	0.767	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.235	0.765	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.689	0.311	0.725	0.275	0.000	64.742	349.953	48.209	8.306
2	0.680	0.320	0.735	0.265	102.252	64.634	349.96	48.273	8.364
3	0.688	0.312	0.748	0.252	102.144	64.577	349.939	48.353	8.433
4	0.704	0.296	0.758	0.242	102.087	64.577	349.911	48.419	8.488
5	0.718	0.282	0.764	0.236	102.087	64.638	349.894	48.453	8.516
6	0.726	0.274	0.762	0.238	102.148	64.765	349.89	48.447	8.511
7	0.723	0.277	0.754	0.246	102.275	64.963	349.897	48.394	8.468
8	0.704	0.296	0.737	0.263	102.473	65.245	349.925	48.29	8.379
9	0.659	0.341	0.712	0.288	102.755	65.684	350.015	48.124	8.224
10	0.559	0.441	0.675	0.325	103.194	66.658	350.331	47.856	7.939
11	0.311	0.689	0.613	0.387	104.168	261.808	351.701	47.304	7.255
12	0.314	0.686	0.614	0.386	103.018	262.072	351.679	47.313	7.267
13	0.290	0.710	0.605	0.395	103.282	262.32	351.881	47.242	7.174
14	0.122	0.878	0.520	0.480	103.53	158.8	354.845	46.910	6.724

Table5.68 Simulation results using %AAD of the K-value = +37.79%. (1.90A_{21})

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.995	0.005	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.990	0.010	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.982	0.018	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.966	0.034	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.937	0.063	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.886	0.114	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.803	0.197	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.68	0.320	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.526	0.474	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.366	0.634	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.233	0.767	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.770	0.230	0.851	0.149	0.000	64.742	354.303	49.535	9.046
2	0.655	0.345	0.771	0.229	102.252	64.987	355.672	49.314	8.852
3	0.556	0.444	0.699	0.301	102.497	65.211	356.945	49.095	8.668
4	0.472	0.528	0.637	0.363	102.721	65.401	358.090	48.890	8.498
5	0.405	0.595	0.585	0.415	102.911	65.554	359.086	48.708	8.348
6	0.352	0.648	0.543	0.457	103.064	65.673	359.924	48.553	8.223
7	0.311	0.689	0.509	0.491	103.183	65.766	360.608	48.427	8.122
8	0.281	0.719	0.483	0.517	103.276	65.838	361.151	48.327	8.042
9	0.258	0.742	0.463	0.537	103.348	65.900	361.573	48.247	7.979
10	0.242	0.758	0.447	0.553	103.410	65.956	361.900	48.184	7.929
11	0.229	0.771	0.433	0.567	103.466	265.429	362.155	48.130	7.888
12	0.214	0.786	0.420	0.58	106.639	265.538	362.458	48.078	7.848
13	0.178	0.822	0.384	0.616	106.748	265.710	363.281	47.937	7.743
14	0.102	0.897	0.293	0.707	106.920	158.800	365.454	47.610	7.524

Table5.69 Simulation results using %AAD of the K-value = -37.58%. (0.55A_{21})

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.996	0.004	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.993	0.007	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.987	0.013	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.974	0.026	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.950	0.05	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.906	0.094	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.828	0.172	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.707	0.293	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.548	0.452	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.377	0.623	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.233	0.767	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.233	0.767	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.235	0.765	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.667	0.333	0.709	0.291	0.000	64.742	349.654	48.047	8.177
2	0.640	0.360	0.716	0.283	102.252	64.581	349.701	48.098	8.228
3	0.644	0.356	0.731	0.269	102.091	64.477	349.683	48.194	8.318
4	0.666	0.334	0.745	0.255	101.987	64.436	349.632	48.291	8.405
5	0.691	0.309	0.756	0.244	101.946	64.460	349.587	48.362	8.464
6	0.711	0.289	0.760	0.240	101.97	64.555	349.566	48.390	8.486
7	0.719	0.281	0.756	0.244	102.065	64.738	349.564	48.367	8.468
8	0.710	0.290	0.743	0.257	102.248	65.029	349.578	48.284	8.398
9	0.674	0.326	0.720	0.280	102.539	65.506	349.635	48.126	8.255
10	0.579	0.421	0.683	0.317	103.016	66.589	349.886	47.852	7.967
11	0.314	0.686	0.620	0.380	104.099	261.484	351.202	47.256	7.225
12	0.316	0.684	0.622	0.378	102.694	261.741	351.186	47.269	7.242
13	0.297	0.703	0.616	0.384	102.951	262.143	351.341	47.213	7.168
14	0.128	0.872	0.538	0.462	103.353	158.800	354.108	46.870	6.693

Table5.70 %AAD of liquid composition (x_1) profile by varying the K-value in increasing Wilson parameter (A_{21}).

Stage	$X_{1accurate}$	$X_{1(+6.66\%)}$	Δ	$X_{1(+9.25\%)}$	Δ	$X_{1(+22.77\%)}$	Δ	$X_{1(+31.74\%)}$	Δ	$X_{1(+37.79\%)}$	Δ
1	0.786	0.804	0.0229	0.807	0.0267	0.812	0.0331	0.797	0.0140	0.770	0.0204
2	0.755	0.775	0.0265	0.773	0.0238	0.748	0.0093	0.707	0.0636	0.655	0.1325
3	0.725	0.747	0.0303	0.741	0.0221	0.688	0.0510	0.625	0.1379	0.556	0.2331
4	0.696	0.720	0.0345	0.709	0.0187	0.630	0.0948	0.551	0.2083	0.472	0.3218
5	0.667	0.690	0.0345	0.676	0.0135	0.574	0.1394	0.484	0.2744	0.405	0.3928
6	0.637	0.656	0.0298	0.639	0.0031	0.517	0.1884	0.424	0.3344	0.352	0.4474
7	0.602	0.614	0.0199	0.595	0.0116	0.462	0.2326	0.373	0.3804	0.311	0.4834
8	0.560	0.560	0.0000	0.539	0.0375	0.407	0.2732	0.329	0.4125	0.281	0.4982
9	0.502	0.488	0.0279	0.468	0.0677	0.353	0.2968	0.292	0.4183	0.258	0.4861
10	0.413	0.392	0.0508	0.377	0.0872	0.300	0.2736	0.261	0.3680	0.242	0.4140
11	0.274	0.270	0.0146	0.266	0.0292	0.245	0.1058	0.234	0.1460	0.229	0.1642
12	0.268	0.259	0.0336	0.254	0.0522	0.233	0.1306	0.220	0.1791	0.214	0.2015
13	0.231	0.211	0.0866	0.208	0.0996	0.193	0.1645	0.181	0.2165	0.178	0.2294
14	0.101	0.088	0.1287	0.089	0.1188	0.094	0.0693	0.097	0.0396	0.102	0.0099
Sum of data			0.5407		0.6118		2.0625		3.1930		4.0347

N = number of data points

$$\Delta = \left| \frac{x_{1at\ \%AAD} - x_{1accurate}}{x_{1accurate}} \right|$$

%Average Absolute Deviation = $\frac{1}{N}\left[\sum_{N} \left| \frac{x_{1at\ \%AAD} - x_{1accurate}}{x_{1accurate}} \right| \right] x100$

At +6.66%AAD of K-value = (0.5407x100)/14

= 3.86%

At +9.25%AAD of K-value = (0.6118x100)/14

= 4.37%

At +22.77%AAD of K-value = (2.0625x100)/14

= 14.73%

At +31.74%AAD of K-value = (3.1930x100)/14

= 22.81%

At +37.79%AAD of K-value = (4.0347x100)/14

= 28.82%

Table5.71 %AAD of liquid composition (x_1) profile by varying the K-value in decreasing Wilson parameter (A_{21}).

Stage	$X_{1accurate}$	$X_{1(-6.30\%)}$	Δ	$X_{1(-9.99\%)}$	Δ	$X_{1(-22.20\%)}$	Δ	$X_{1(-32.04\%)}$	Δ	$X_{1(-37.58\%)}$	Δ
1	0.7860	0.794	0.0102	0.785	0.0013	0.724	0.0789	0.689	0.1234	0.667	0.1514
2	0.7550	0.776	0.0278	0.777	0.0291	0.715	0.0530	0.680	0.0993	0.640	0.1523
3	0.7250	0.756	0.0428	0.765	0.0552	0.712	0.0179	0.688	0.0510	0.644	0.1117
4	0.6960	0.732	0.0517	0.749	0.0761	0.712	0.0230	0.704	0.0115	0.666	0.0431
5	0.6670	0.705	0.0570	0.729	0.0930	0.711	0.0660	0.718	0.0765	0.691	0.0360
6	0.6370	0.674	0.0581	0.702	0.1020	0.706	0.1083	0.726	0.1397	0.711	0.1162
7	0.6020	0.637	0.0581	0.668	0.1096	0.692	0.1495	0.723	0.2010	0.719	0.1944
8	0.5600	0.591	0.0554	0.622	0.1107	0.666	0.1893	0.704	0.2571	0.710	0.2679
9	0.5020	0.529	0.0538	0.559	0.1135	0.617	0.2291	0.659	0.3127	0.674	0.3426
10	0.4130	0.435	0.0533	0.459	0.1114	0.519	0.2567	0.559	0.3535	0.579	0.4019
11	0.2740	0.278	0.0146	0.286	0.0438	0.303	0.1058	0.311	0.1350	0.314	0.1460
12	0.2680	0.268	0.0000	0.277	0.0336	0.304	0.1343	0.314	0.1716	0.316	0.1791
13	0.2310	0.226	0.0216	0.233	0.0087	0.274	0.1861	0.290	0.2554	0.297	0.2857
14	0.1010	0.094	0.0693	0.093	0.0792	0.113	0.1188	0.122	0.2079	0.128	0.2673
Sum of data			0.5736		0.9672		1.7167		2.3959		2.6956

N = number of data points

$$\Delta = \left| \frac{x_{1at\ \%AAD} - x_{1accurate}}{x_{1accurate}} \right|$$

%Average Absolute Deviation = $\frac{1}{N}\left[\sum_{N} \left| \frac{x_{1at\ \%AAD} - x_{1accurate}}{x_{1accurate}} \right| \right]$x100

At –6.30%AAD of K-value = (0.5736x100)/14

= 4.10%

At –9.99%AAD of K-value = (0.9672x100)/14

= 6.91%

At –22.20%AAD of K-value = (1.7167x100)/14

= 12.26%

At –32.04%AAD of K-value = (2.3959x100)/14

= 17.11%

At –37.58%AAD of K-value = (2.6956x100)/14

= 19.25%

Table5.72 %AAD of temperature profile by varying the K-value in increasing Wilson parameter (A_{21}).

Stage	$T_{accurate}$	$T_{(+6.66\%)}$	Δ	$T_{(+9.25\%)}$	Δ	$T_{(+22.77\%)}$	Δ	$T_{(+31.74\%)}$	Δ	$T_{(+37.79\%)}$	Δ
1	351.827	352.110	0.0008	352.255	0.0012	353.009	0.0034	353.643	0.0052	354.303	0.0070
2	351.921	352.221	0.0009	352.403	0.0014	353.487	0.0044	354.541	0.0074	355.672	0.0107
3	352.028	352.339	0.0009	352.557	0.0015	353.968	0.0055	355.414	0.0096	356.945	0.0140
4	352.147	352.470	0.0009	352.724	0.0016	354.467	0.0066	356.262	0.0117	358.090	0.0169
5	352.282	352.623	0.0010	352.915	0.0018	354.995	0.0077	357.082	0.0136	359.086	0.0193
6	352.439	352.817	0.0011	353.149	0.0020	355.559	0.0089	357.863	0.0154	359.924	0.0212
7	352.634	353.079	0.0013	353.454	0.0023	356.162	0.0100	358.593	0.0169	360.608	0.0226
8	352.898	353.454	0.0016	353.873	0.0028	356.805	0.0111	359.261	0.0180	361.151	0.0234
9	353.304	354.017	0.0020	354.476	0.0033	357.493	0.0119	359.861	0.0186	361.573	0.0234
10	354.027	354.893	0.0024	355.372	0.0038	358.256	0.0119	360.404	0.0180	361.900	0.0222
11	355.505	356.326	0.0023	356.752	0.0035	359.161	0.0103	360.906	0.0152	362.155	0.0187
12	355.582	356.488	0.0025	356.923	0.0038	359.371	0.0107	361.183	0.0158	362.458	0.0193
13	356.110	357.253	0.0032	357.704	0.0045	360.171	0.0114	362.032	0.0166	363.281	0.0201
14	359.443	360.864	0.0040	361.239	0.0050	363.108	0.0102	364.562	0.0142	365.454	0.0167
Sum of data			0.0248		0.0385		0.1239		0.1962		0.2556

N = number of data points

$$\Delta = \left| \frac{T_{at\ \%AAD} - T_{accurate}}{T_{accurate}} \right|$$

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N} \left| \frac{T_{at\ \%AAD} - T_{accurate}}{T_{accurate}} \right| \right] x100$$

At +6.66%AAD of K-value = (0.0248x100)/14

= 0.18%

At +9.25%AAD of K-value = (0.0385x100)/14

= 0.28%

At +22.77%AAD of K-value = (0.1239x100)/14

= 0.89%

At +31.74%AAD of K-value = (0.1962x100)/14

= 1.40%

At +37.79%AAD of K-value = (0.2556x100)/14

= 1.83%

Table5.73 %AAD of temperature profile by varying the K-value in decreasing Wilson parameter (A_{21}).

Stage	$T_{accurate}$	$T_{(-6.30\%)}$	Δ	$T_{(-9.99\%)}$	Δ	$T_{(-22.20\%)}$	Δ	$T_{(-32.04\%)}$	Δ	$T_{(-37.58\%)}$	Δ
1	351.827	351.415	0.0012	351.205	0.0018	350.517	0.0037	349.953	0.0053	349.654	0.0062
2	351.921	351.449	0.0013	351.220	0.0020	350.526	0.0040	349.960	0.0056	349.701	0.0063
3	352.028	351.496	0.0015	351.242	0.0022	350.527	0.0043	349.939	0.0059	349.683	0.0067
4	352.147	351.559	0.0017	351.275	0.0025	350.526	0.0046	349.911	0.0063	349.632	0.0071
5	352.282	351.645	0.0018	351.325	0.0027	350.528	0.0050	349.894	0.0068	349.587	0.0077
6	352.439	351.763	0.0019	351.402	0.0029	350.541	0.0054	349.890	0.0072	349.566	0.0082
7	352.634	351.924	0.0020	351.521	0.0032	350.572	0.0058	349.897	0.0078	349.564	0.0087
8	352.898	352.155	0.0021	351.711	0.0034	350.643	0.0064	349.925	0.0084	349.578	0.0094
9	353.304	352.515	0.0022	352.032	0.0036	350.807	0.0071	350.015	0.0093	349.635	0.0104
10	354.027	353.172	0.0024	352.652	0.0039	351.239	0.0079	350.331	0.0104	349.886	0.0117
11	355.505	354.663	0.0024	354.152	0.0038	352.691	0.0079	351.701	0.0107	351.202	0.0121
12	355.582	354.788	0.0022	354.256	0.0037	352.681	0.0082	351.679	0.0110	351.186	0.0124
13	356.110	355.354	0.0021	354.824	0.0036	352.978	0.0088	351.881	0.0119	351.341	0.0134
14	359.443	358.888	0.0015	358.488	0.0027	356.173	0.0091	354.845	0.0128	354.108	0.0148
Sum of data			0.0265		0.0419		0.0881		0.1195		0.1350

N = number of data points

$$\Delta = \left| \frac{T_{at\ \%AAD} - T_{accurate}}{T_{accurate}} \right|$$

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\frac{T_{at\ \%AAD} - T_{accurate}}{T_{accurate}}\right|\right]x100$$

At –6.30%AAD of K-value = (0.0265x100)/14

= 0.19%

At –9.99%AAD of K-value = (0.0419x100)/14

= 0.30%

At –22.20%AAD of K-value = (0.0881x100)/14

= 0.63%

At –32.04%AAD of K-value = (0.1195x100)/14

= 0.85%

At –37.58%AAD of K-value = (0.1350x100)/14

= 0.96%

Table5.74 Simulation results using %AAD of the enthalpy model = +23%. (1.05D_1)

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.994	0.006	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.989	0.011	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.980	0.020	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.963	0.037	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.932	0.068	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.879	0.121	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.793	0.207	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.670	0.33	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.519	0.481	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.363	0.637	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.234	0.766	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.780	0.220	0.804	0.196	0.000	64.742	351.84	44.338	6.497
2	0.750	0.250	0.787	0.213	102.252	64.659	351.931	44.378	6.507
3	0.723	0.277	0.772	0.228	102.169	64.576	352.029	44.415	6.517
4	0.698	0.302	0.759	0.241	102.086	64.487	352.135	44.452	6.526
5	0.672	0.328	0.745	0.255	101.997	64.382	352.254	44.491	6.537
6	0.644	0.356	0.730	0.270	101.892	64.246	352.395	44.537	6.550
7	0.611	0.389	0.711	0.289	101.756	64.056	352.579	44.596	6.566
8	0.568	0.432	0.688	0.312	101.566	63.78	352.843	44.677	6.588
9	0.507	0.493	0.656	0.344	101.29	63.377	353.269	44.795	6.618
10	0.413	0.587	0.612	0.388	100.887	62.812	354.032	44.967	6.657
11	0.274	0.726	0.552	0.448	100.322	259.483	355.505	45.207	6.694
12	0.269	0.731	0.549	0.451	100.693	259.285	355.569	45.217	6.696
13	0.231	0.769	0.528	0.472	100.495	258.35	356.117	45.297	6.706
14	0.100	0.900	0.424	0.576	99.560	158.800	359.467	45.685	6.799

Table5.75 Simulation results using %AAD of the enthalpy model = -23%. (0.99D_1)

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.994	0.006	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.989	0.011	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.980	0.020	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.963	0.037	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.932	0.068	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.879	0.121	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.793	0.207	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.670	0.330	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.519	0.481	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.363	0.637	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.234	0.766	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.786	0.214	0.800	0.200	0.000	64.742	351.827	49.844	9.2081
2	0.755	0.245	0.781	0.219	102.252	64.865	351.922	49.72	9.116
3	0.725	0.275	0.764	0.236	102.375	64.977	352.028	49.614	9.035
4	0.696	0.304	0.749	0.251	102.487	65.089	352.147	49.518	8.960
5	0.667	0.333	0.735	0.265	102.599	65.21	352.282	49.426	8.885
6	0.637	0.363	0.720	0.280	102.72	65.356	352.438	49.331	8.807
7	0.603	0.397	0.704	0.296	102.866	65.555	352.632	49.223	8.714
8	0.561	0.439	0.684	0.316	103.065	65.852	352.893	49.087	8.593
9	0.503	0.497	0.656	0.344	103.362	66.329	353.295	48.894	8.415
10	0.415	0.585	0.616	0.384	103.839	67.073	354.013	48.595	8.122
11	0.275	0.725	0.554	0.446	104.583	263.85	355.496	48.121	7.636
12	0.269	0.731	0.552	0.448	105.060	264.112	355.569	48.110	7.624
13	0.232	0.768	0.534	0.466	105.322	264.445	356.095	47.979	7.489
14	0.101	0.899	0.431	0.569	105.655	158.800	359.435	47.515	7.062

Table5.76 Simulation results using %AAD of the enthalpy model = +28%. (1.06D_1)

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.994	0.006	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.989	0.011	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.980	0.020	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.963	0.037	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.932	0.068	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.879	0.121	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.793	0.207	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.670	0.330	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.519	0.481	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.363	0.637	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.234	0.766	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.780	0.220	0.804	0.196	0	64.742	351.839	43.417	6.043
2	0.750	0.250	0.787	0.213	102.252	64.622	351.93	43.482	6.068
3	0.723	0.277	0.772	0.228	102.132	64.504	352.029	43.541	6.091
4	0.698	0.302	0.758	0.242	102.014	64.376	352.136	43.600	6.113
5	0.672	0.328	0.744	0.256	101.886	64.225	352.256	43.661	6.138
6	0.643	0.357	0.729	0.271	101.735	64.031	352.4	43.732	6.166
7	0.610	0.390	0.710	0.290	101.541	63.762	352.586	43.822	6.203
8	0.567	0.433	0.686	0.314	101.272	63.376	352.854	43.945	6.252
9	0.505	0.495	0.654	0.346	100.886	62.82	353.286	44.120	6.323
10	0.410	0.590	0.611	0.389	100.33	62.056	354.054	44.375	6.420
11	0.273	0.727	0.551	0.449	99.566	258.705	355.521	44.727	6.541
12	0.268	0.732	0.549	0.451	99.915	258.438	355.587	44.743	6.546
13	0.230	0.770	0.528	0.472	99.648	257.331	356.136	44.858	6.582
14	0.100	0.900	0.424	0.576	98.541	158.800	359.474	45.383	6.757

Table5.77 Simulation results using %AAD of the enthalpy model = -28%. (0.97D_1)

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.994	0.006	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.989	0.011	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.980	0.020	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.963	0.037	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.932	0.068	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.879	0.121	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.793	0.207	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.670	0.33	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.519	0.481	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.363	0.637	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.234	0.766	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.786	0.214	0.800	0.200	0.000	64.742	351.827	51.673	10.108
2	0.755	0.245	0.780	0.220	102.252	64.930	351.922	51.492	9.982
3	0.725	0.275	0.764	0.236	102.44	65.102	352.029	51.337	9.871
4	0.696	0.304	0.749	0.251	102.612	65.273	352.148	51.196	9.768
5	0.667	0.333	0.735	0.265	102.783	65.458	352.282	51.062	9.667
6	0.637	0.363	0.721	0.279	102.968	65.683	352.437	50.924	9.560
7	0.603	0.397	0.705	0.295	103.193	65.987	352.628	50.766	9.435
8	0.562	0.438	0.685	0.315	103.497	66.447	352.885	50.565	9.271
9	0.505	0.495	0.658	0.342	103.957	67.197	353.279	50.279	9.029
10	0.418	0.582	0.618	0.382	104.707	68.405	353.988	49.829	8.630
11	0.276	0.724	0.555	0.445	105.915	265.221	355.477	49.107	7.960
12	0.271	0.729	0.554	0.446	106.431	265.649	355.546	49.092	7.947
13	0.234	0.766	0.535	0.465	106.859	266.444	356.066	48.893	7.763
14	0.101	0.899	0.431	0.569	107.654	158.8	359.419	48.136	7.153

Table5.78 Simulation results using %AAD of the enthalpy model = +33%. (1.07D_1)

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.994	0.006	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.989	0.011	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.980	0.020	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.963	0.037	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.932	0.068	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.879	0.121	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.793	0.207	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.670	0.330	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.519	0.481	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.363	0.637	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.234	0.766	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.780	0.220	0.804	0.196	0.000	64.742	351.839	42.496	5.589
2	0.750	0.250	0.786	0.214	102.252	64.585	351.93	42.587	5.629
3	0.723	0.277	0.772	0.228	102.095	64.428	352.029	42.669	5.665
4	0.697	0.303	0.758	0.242	101.938	64.26	352.137	42.749	5.702
5	0.671	0.329	0.744	0.256	101.77	64.062	352.259	42.833	5.740
6	0.643	0.357	0.728	0.272	101.572	63.807	352.404	42.93	5.785
7	0.609	0.391	0.709	0.291	101.317	63.458	352.593	43.052	5.842
8	0.565	0.435	0.685	0.315	100.968	62.96	352.865	43.216	5.920
9	0.503	0.497	0.653	0.347	100.47	62.252	353.302	43.450	6.030
10	0.408	0.592	0.610	0.390	99.762	61.297	354.073	43.785	6.186
11	0.273	0.727	0.551	0.449	98.807	258.438	355.527	44.247	6.388
12	0.267	0.733	0.548	0.452	99.648	258.101	355.596	44.268	6.397
13	0.229	0.771	0.528	0.472	99.311	256.817	356.148	44.42	6.459
14	0.100	0.900	0.424	0.576	98.027	158.8	359.479	45.08	6.715

Table5.79 Simulation results using %AAD of the enthalpy model = -33%. (0.95D_1)

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.994	0.006	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.989	0.011	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.980	0.020	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.963	0.037	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.932	0.068	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.879	0.121	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.793	0.207	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.670	0.330	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.519	0.481	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.363	0.637	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.234	0.766	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.786	0.214	0.799	0.201	0.000	64.742	351.827	53.498	11.006
2	0.755	0.245	0.780	0.220	102.252	64.991	351.923	53.261	10.846
3	0.725	0.275	0.763	0.237	102.501	65.219	352.03	53.057	10.705
4	0.696	0.304	0.749	0.251	102.729	65.444	352.149	52.874	10.575
5	0.667	0.333	0.735	0.265	102.954	65.688	352.282	52.699	10.448
6	0.637	0.363	0.721	0.279	103.198	65.984	352.436	52.519	10.314
7	0.604	0.396	0.706	0.294	103.494	66.387	352.625	52.313	10.158
8	0.563	0.437	0.686	0.314	103.897	67.000	352.878	52.051	9.954
9	0.507	0.493	0.660	0.340	104.510	68.015	353.265	51.674	9.650
10	0.420	0.580	0.619	0.381	105.525	69.697	353.966	51.077	9.147
11	0.278	0.722	0.556	0.444	107.207	266.556	355.458	50.100	8.291
12	0.273	0.727	0.555	0.445	107.766	267.16	355.522	50.084	8.277
13	0.236	0.764	0.536	0.464	108.370	268.44	356.036	49.816	8.043
14	0.102	0.898	0.432	0.568	109.650	158.800	359.402	48.760	7.246

Table5.80 Simulation results using %AAD of the enthalpy model = +37%. (1.08D_1)

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.994	0.006	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.989	0.011	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.980	0.020	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.963	0.037	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.932	0.068	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.879	0.121	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.793	0.207	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.670	0.330	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.519	0.481	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.363	0.637	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.234	0.766	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.780	0.220	0.804	0.196	0.000	64.742	351.838	41.575	5.135
2	0.751	0.249	0.786	0.214	102.252	64.544	351.93	41.692	5.190
3	0.723	0.277	0.771	0.229	102.054	64.348	352.03	41.797	5.241
4	0.697	0.303	0.757	0.243	101.858	64.136	352.138	41.900	5.291
5	0.671	0.329	0.743	0.257	101.646	63.887	352.262	42.008	5.344
6	0.642	0.358	0.727	0.273	101.397	63.568	352.409	42.132	5.406
7	0.607	0.393	0.708	0.292	101.078	63.134	352.602	42.287	5.485
8	0.563	0.437	0.684	0.316	100.644	62.522	352.879	42.495	5.592
9	0.500	0.500	0.651	0.349	100.032	61.661	353.323	42.789	5.743
10	0.405	0.595	0.608	0.392	99.171	60.519	354.102	43.206	5.958
11	0.271	0.729	0.550	0.450	98.029	257.13	355.551	43.774	6.239
12	0.265	0.735	0.547	0.453	98.340	256.732	355.623	43.801	6.252
13	0.228	0.772	0.527	0.473	97.942	255.296	356.174	43.987	6.338
14	0.100	0.900	0.424	0.576	96.506	158.800	359.487	44.776	6.673

Table5.81 Simulation results using %AAD of the enthalpy model = -37%. (0.94D_1)

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.994	0.006	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.989	0.011	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.980	0.020	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.963	0.037	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.932	0.068	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.879	0.121	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.793	0.207	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.670	0.330	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.519	0.481	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.363	0.637	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.234	0.766	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.786	0.214	0.799	0.201	0.000	64.742	351.828	54.410	11.454
2	0.754	0.246	0.78	0.220	102.252	65.020	351.923	54.145	11.278
3	0.725	0.275	0.763	0.237	102.530	65.274	352.031	53.917	11.122
4	0.696	0.304	0.749	0.251	102.784	65.525	352.150	53.712	10.978
5	0.667	0.333	0.735	0.265	103.035	65.797	352.283	53.517	10.839
6	0.637	0.363	0.721	0.279	103.307	66.126	352.436	53.317	10.692
7	0.604	0.396	0.706	0.294	103.636	66.575	352.623	53.088	10.521
8	0.563	0.437	0.687	0.313	104.085	67.261	352.874	52.796	10.297
9	0.508	0.492	0.660	0.340	104.771	68.406	353.259	52.375	9.963
10	0.421	0.579	0.620	0.380	105.916	70.328	353.955	51.705	9.409
11	0.278	0.722	0.557	0.443	107.838	267.210	355.450	50.599	8.458
12	0.274	0.726	0.556	0.444	108.420	267.906	355.510	50.583	8.444
13	0.237	0.763	0.537	0.463	109.116	269.437	356.021	50.280	8.186
14	0.102	0.898	0.432	0.568	110.647	158.800	359.394	49.072	7.293

Table5.82 %AAD of liquid composition (x_1) profile by varying the enthalpy model in increasing constant (D_1).

Stage	$X_{1accurate}$	$X_{1(+23..18\%)}$	Δ	$X_{1(+27.72\%)}$	Δ	$X_{1(+32.99\%)}$	Δ	$X_{1(+37.98\%)}$	Δ
1	0.786	0.780	0.0076	0.780	0.0076	0.780	0.0076	0.780	0.0076
2	0.755	0.750	0.0066	0.750	0.0066	0.750	0.0066	0.751	0.0053
3	0.725	0.723	0.0028	0.723	0.0028	0.723	0.0028	0.723	0.0028
4	0.696	0.698	0.0029	0.698	0.0029	0.697	0.0014	0.697	0.0014
5	0.667	0.672	0.0075	0.672	0.0075	0.671	0.0060	0.671	0.0060
6	0.637	0.644	0.0110	0.643	0.0094	0.643	0.0094	0.642	0.0078
7	0.602	0.611	0.0150	0.610	0.0133	0.609	0.0116	0.607	0.0083
8	0.560	0.568	0.0143	0.567	0.0125	0.565	0.0089	0.563	0.0054
9	0.502	0.507	0.0100	0.505	0.0060	0.503	0.0020	0.500	0.0040
10	0.413	0.413	0.0000	0.410	0.0073	0.408	0.0121	0.405	0.0194
11	0.274	0.274	0.0000	0.273	0.0036	0.273	0.0036	0.271	0.0109
12	0.268	0.269	0.0037	0.268	0.0000	0.267	0.0037	0.265	0.0112
13	0.231	0.231	0.0000	0.230	0.0043	0.229	0.0087	0.228	0.0130
14	0.101	0.100	0.0099	0.100	0.0099	0.100	0.0099	0.100	0.0099
Sum of data			0.0912		0.0937		0.0945		0.1130

N = number of data points

$$\Delta = \left| \frac{x_{1at\ \%AAD} - x_{1accurate}}{x_{1accurate}} \right|$$

%Average Absolute Deviation = $\frac{1}{N}\left[\sum_{N}\left|\frac{x_{1at\ \%AAD} - x_{1accurate}}{x_{1accurate}}\right|\right]$x100

At +23.18%AAD of enthalpy = (0.0912x100)/14

= 0.65%

At +27.72%AAD of enthalpy = (0.0937x100)/14

= 0.67%

At +32.99%AAD of enthalpy = (0.0945x100)/14

= 0.68%

At +37.98%AAD of enthalpy = (0.1130x100)/14

= 0.81%

Table5.83 %AAD of liquid composition (x_1) profile by varying the enthalpy model in decreasing constant (D_1).

Stage	$X_{1accurate}$	$X_{1(-23.21\%)}$	Δ	$X_{1(-28.05\%)}$	Δ	$X_{1(-33.42\%)}$	Δ	$X_{1(-36.34\%)}$	Δ
1	0.786	0.786	0.0000	0.786	0.0000	0.786	0.0000	0.786	0.0000
2	0.755	0.755	0.0000	0.755	0.0000	0.755	0.0000	0.754	0.0013
3	0.725	0.725	0.0000	0.725	0.0000	0.725	0.0000	0.725	0.0000
4	0.696	0.696	0.0000	0.696	0.0000	0.696	0.0000	0.696	0.0000
5	0.667	0.667	0.0000	0.667	0.0000	0.667	0.0000	0.667	0.0000
6	0.637	0.637	0.0000	0.637	0.0000	0.637	0.0000	0.637	0.0000
7	0.602	0.603	0.0017	0.603	0.0017	0.604	0.0033	0.604	0.0033
8	0.560	0.561	0.0018	0.562	0.0036	0.563	0.0054	0.563	0.0054
9	0.502	0.503	0.0020	0.505	0.0060	0.507	0.0100	0.508	0.0120
10	0.413	0.415	0.0048	0.418	0.0121	0.42	0.0169	0.421	0.0194
11	0.274	0.275	0.0036	0.276	0.0073	0.278	0.0146	0.278	0.0146
12	0.268	0.269	0.0037	0.271	0.0112	0.273	0.0187	0.274	0.0224
13	0.231	0.232	0.0043	0.234	0.0130	0.236	0.0216	0.237	0.0260
14	0.101	0.101	0.0000	0.101	0.0000	0.102	0.0099	0.102	0.0099
Sum of data			0.0220		0.0548		0.1004		0.1142

N = number of data points

$$\Delta = \left| \frac{x_{1at\ \%AAD} - x_{1accurate}}{x_{1accurate}} \right|$$

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\frac{x_{1at\ \%AAD} - x_{1accurate}}{x_{1accurate}}\right|\right] x100$$

At –23.21%AAD of enthalpy = (0.0220x100)/14

= 0.16%

At –28.05%AAD of enthalpy = (0.0548x100)/14

= 0.39%

At –33.42%AAD of enthalpy = (0.0945x100)/14

= 0.68%

At –36.34%AAD of enthalpy = (0.1004x100)/14

= 0.72%

Table5.84 %AAD of temperature profile by varying the enthalpy model in increasing constant (D_1).

Stage	$T_{accurate}$	$T_{(+23.18\%)}$	Δ	$T_{(+27.72\%)}$	Δ	$T_{(+32.99\%)}$	Δ	$T_{(+3798\%)}$	Δ
1	351.827	351.840	0.00004	351.839	0.00003	351.839	0.00003	351.838	0.00003
2	351.921	351.931	0.00003	351.930	0.00003	351.930	0.00003	351.930	0.00003
3	352.028	352.029	0.00000	352.029	0.00000	352.029	0.00000	352.030	0.00001
4	352.147	352.135	0.00003	352.136	0.00003	352.137	0.00003	352.138	0.00003
5	352.282	352.254	0.00008	352.256	0.00007	352.259	0.00007	352.262	0.00006
6	352.439	352.395	0.00012	352.400	0.00011	352.404	0.00010	352.409	0.00009
7	352.634	352.579	0.00016	352.586	0.00014	352.593	0.00012	352.602	0.00009
8	352.898	352.843	0.00016	352.854	0.00012	352.865	0.00009	352.879	0.00005
9	353.304	353.269	0.00010	353.286	0.00005	353.302	0.00001	353.323	0.00005
10	354.027	354.032	0.00001	354.054	0.00008	354.073	0.00013	354.102	0.00021
11	355.505	355.505	0.00000	355.521	0.00005	355.527	0.00006	355.551	0.00013
12	355.582	355.569	0.00004	355.587	0.00001	355.596	0.00004	355.623	0.00012
13	356.110	356.117	0.00002	356.136	0.00007	356.148	0.00011	356.174	0.00018
14	359.443	359.467	0.00007	359.474	0.00009	359.479	0.00010	359.487	0.00012
Sum of data			0.00085		0.00088		0.00091		0.00119

N = number of data points

$$\Delta = \left| \frac{T_{at\ \%AAD} - T_{accurate}}{T_{accurate}} \right|$$

%Average Absolute Deviation = $\frac{1}{N}\left[\sum_{N} \left| \frac{T_{at\ \%AAD} - T_{accurate}}{T_{accurate}} \right| \right] x100$

At +23.18%AAD of enthalpy = (0.0220x100)/14

= 0.16%

At +27.72%AAD of enthalpy = (0.0548x100)/14

= 0.39%

At +32.99%AAD of enthalpy = (0.0945x100)/14

= 0.68%

At +37.98%AAD of enthalpy = (0.1004x100)/14

= 0.72%

Table5.85 %AAD of temperature profile by varying the enthalpy model in decreasing constant (D_1).

Stage	$T_{accurate}$	$T_{(-23.21\%)}$	Δ	$T_{(-28.05\%)}$	Δ	$T_{(-33.42\%)}$	Δ	$T_{(-36.34\%)}$	Δ
1	351.827	351.827	0.00000	351.827	0.00000	351.827	0.00000	351.828	0.00000
2	351.921	351.922	0.00000	351.922	0.00000	351.923	0.00001	351.923	0.00001
3	352.028	352.028	0.00000	352.029	0.00000	352.030	0.00001	352.031	0.00001
4	352.147	352.147	0.00000	352.148	0.00000	352.149	0.00001	352.150	0.00001
5	352.282	352.282	0.00000	352.282	0.00000	352.282	0.00000	352.283	0.00000
6	352.439	352.438	0.00000	352.437	0.00001	352.436	0.00001	352.436	0.00001
7	352.634	352.632	0.00001	352.628	0.00002	352.625	0.00003	352.623	0.00003
8	352.898	352.893	0.00001	352.885	0.00004	352.878	0.00006	352.874	0.00007
9	353.304	353.295	0.00003	353.279	0.00007	353.265	0.00011	353.259	0.00013
10	354.027	354.013	0.00004	353.988	0.00011	353.966	0.00017	353.955	0.00020
11	355.505	355.496	0.00003	355.477	0.00008	355.458	0.00013	355.450	0.00015
12	355.582	355.569	0.00004	355.546	0.00010	355.522	0.00017	355.510	0.00020
13	356.110	356.095	0.00004	356.066	0.00012	356.036	0.00021	356.021	0.00025
14	359.443	359.435	0.00002	359.419	0.00007	359.402	0.00011	359.394	0.00014
Sum of data			0.00022		0.00062		0.00101		0.00121

N = number of data points

$$\Delta = \left| \frac{T_{at\ \%AAD} - T_{accurate}}{T_{accurate}} \right|$$

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N} \left| \frac{T_{at\ \%AAD} - T_{accurate}}{T_{accurate}} \right| \right] x100$$

At –23.21%AAD of enthalpy = (0.00022x100)/14
= 0.002%

At –28.05%AAD of enthalpy = (0.00062x100)/14
= 0.004%

At –33.42%AAD of enthalpy = (0.00101x100)/14
= 0.007%

At –36.34%AAD of enthalpy = (0.00121x100)/14
= 0.009%

Table5.86 Simulation results using reflux ratio r =1.9.

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.994	0.006	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.989	0.011	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.980	0.020	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.963	0.037	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.932	0.068	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.879	0.121	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.793	0.207	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.670	0.330	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.519	0.481	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.363	0.637	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.234	0.766	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.793	0.207	0.803	0.197	0.000	71.216	351.811	48.939	8.765
2	0.763	0.236	0.784	0.216	108.726	71.308	351.895	48.846	8.693
3	0.735	0.265	0.767	0.233	108.818	71.391	351.993	48.766	8.629
4	0.706	0.294	0.752	0.248	108.901	71.473	352.106	48.693	8.568
5	0.677	0.323	0.738	0.262	108.983	71.560	352.236	48.623	8.508
6	0.646	0.354	0.723	0.277	109.070	71.665	352.391	48.551	8.445
7	0.611	0.389	0.707	0.293	109.175	71.805	352.583	48.472	8.372
8	0.569	0.431	0.688	0.312	109.315	72.017	352.842	48.372	8.278
9	0.511	0.489	0.661	0.339	109.527	72.368	353.236	48.233	8.139
10	0.423	0.577	0.621	0.379	109.878	72.951	353.941	48.014	7.906
11	0.279	0.721	0.557	0.443	110.461	269.724	355.437	47.650	7.497
12	0.273	0.727	0.556	0.444	110.934	269.945	355.516	47.643	7.488
13	0.235	0.765	0.536	0.464	111.155	270.100	356.057	47.542	7.373
14	0.100	0.900	0.431	0.569	111.310	158.800	359.466	47.206	7.017

Table5.87 Simulation results using reflux ratio r=1.9 and %AAD of K-value = +9.25%.

Initiated data:

Stage	X_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.993	0.007	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.988	0.012	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.979	0.021	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.961	0.039	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.930	0.070	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.875	0.124	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.789	0.211	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.666	0.334	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.516	0.484	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.362	0.638	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.234	0.766	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.814	0.186	0.844	0.156	0.000	71.216	352.227	49.205	8.929
2	0.783	0.217	0.821	0.179	108.726	71.335	352.357	49.104	8.854
3	0.754	0.246	0.800	0.200	108.845	71.458	352.493	49.012	8.783
4	0.724	0.276	0.779	0.221	108.968	71.591	352.643	48.920	8.710
5	0.693	0.307	0.757	0.243	109.101	71.742	352.816	48.823	8.630
6	0.658	0.342	0.733	0.267	109.252	71.919	353.029	48.715	8.537
7	0.616	0.384	0.705	0.295	109.429	72.130	353.308	48.589	8.425
8	0.562	0.438	0.673	0.327	109.640	72.380	353.699	48.438	8.284
9	0.490	0.510	0.634	0.366	109.890	72.686	354.280	48.254	8.102
10	0.395	0.605	0.589	0.411	110.196	73.067	355.182	48.023	7.862
11	0.273	0.727	0.530	0.470	110.577	270.323	356.648	47.727	7.544
12	0.260	0.740	0.522	0.478	111.533	270.390	356.838	47.687	7.501
13	0.209	0.791	0.494	0.506	111.600	270.320	357.675	47.559	7.365
14	0.086	0.914	0.380	0.620	111.530	158.800	361.361	47.255	7.092

Table5.88 Simulation results using reflux ratio r=1.9 and %AAD of K-value = -9.99%.

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.994	0.006	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.990	0.010	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.981	0.019	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.965	0.035	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.936	0.064	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.884	0.116	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.800	0.200	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.678	0.322	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.524	0.476	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.366	0.634	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.233	0.767	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.234	0.766	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.770	0.230	0.775	0.225	0.000	71.216	351.236	48.704	8.626
2	0.748	0.252	0.764	0.236	108.726	71.262	351.274	48.648	8.581
3	0.728	0.272	0.756	0.244	108.772	71.308	351.320	48.601	8.542
4	0.708	0.292	0.748	0.252	108.818	71.359	351.372	48.559	8.507
5	0.689	0.311	0.740	0.260	108.869	71.426	351.433	48.517	8.471
6	0.668	0.332	0.731	0.269	108.936	71.519	351.508	48.469	8.428
7	0.643	0.357	0.720	0.280	109.029	71.657	351.607	48.407	8.372
8	0.609	0.391	0.704	0.296	109.167	71.875	351.759	48.320	8.290
9	0.558	0.442	0.680	0.320	109.385	72.257	352.025	48.186	8.157
10	0.468	0.532	0.643	0.357	109.767	72.993	352.587	47.960	7.914
11	0.292	0.708	0.578	0.422	110.503	269.192	354.089	47.534	7.415
12	0.288	0.712	0.577	0.423	110.402	269.411	354.135	47.530	7.410
13	0.252	0.748	0.562	0.438	110.621	269.582	354.564	47.439	7.300
14	0.105	0.895	0.464	0.536	110.792	158.800	357.943	47.110	6.914

Table5.89 Simulation results using reflux ratio r=1.9 and %AAD of K-value = +22.77%.

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.993	0.006	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.988	0.012	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.979	0.021	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.961	0.039	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.930	0.070	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.876	0.124	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.790	0.210	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.667	0.333	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.516	0.484	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.362	0.638	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.234	0.766	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.826	0.174	0.864	0.136	0.000	71.216	352.911	49.409	9.027
2	0.768	0.232	0.822	0.178	108.726	71.388	353.333	49.257	8.906
3	0.713	0.287	0.784	0.216	108.898	71.555	353.764	49.114	8.791
4	0.659	0.341	0.747	0.253	109.065	71.719	354.217	48.976	8.675
5	0.604	0.396	0.711	0.289	109.229	71.879	354.704	48.840	8.558
6	0.549	0.451	0.677	0.323	109.389	72.036	355.237	48.704	8.437
7	0.492	0.508	0.643	0.357	109.546	72.191	355.826	48.568	8.313
8	0.434	0.566	0.610	0.390	109.701	72.357	356.480	48.429	8.184
9	0.375	0.625	0.576	0.424	109.867	72.555	357.210	48.284	8.047
10	0.314	0.686	0.539	0.461	110.065	72.811	358.051	48.121	7.892
11	0.249	0.751	0.494	0.506	110.321	271.080	359.080	47.926	7.706
12	0.236	0.764	0.486	0.514	112.290	271.262	359.306	47.894	7.676
13	0.193	0.807	0.452	0.548	112.472	271.363	360.166	47.756	7.549
14	0.091	0.909	0.343	0.657	112.573	158.800	363.246	47.413	7.279

Table5.90 Simulation results using reflux ratio r=1.9 and %AAD of K-value =-22.20%.

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.995	0.005	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.991	0.009	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.984	0.016	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.969	0.031	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.942	0.058	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.893	0.107	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.812	0.188	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.690	0.310	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.534	0.466	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.371	0.629	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.233	0.767	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.233	0.767	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.235	0.765	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.765	0.235	0.778	0.222	0.000	71.216	350.471	48.618	8.608
2	0.775	0.225	0.780	0.220	108.726	71.298	350.472	48.631	8.618
3	0.779	0.221	0.776	0.224	108.808	71.410	350.477	48.608	8.600
4	0.776	0.224	0.766	0.234	108.920	71.536	350.482	48.555	8.559
5	0.765	0.235	0.754	0.246	109.046	71.665	350.488	48.481	8.499
6	0.746	0.254	0.739	0.261	109.175	71.792	350.504	48.395	8.425
7	0.719	0.281	0.724	0.276	109.302	71.930	350.540	48.300	8.340
8	0.681	0.319	0.706	0.294	109.440	72.118	350.620	48.194	8.239
9	0.624	0.376	0.686	0.314	109.628	72.465	350.792	48.059	8.102
10	0.525	0.475	0.655	0.345	109.975	73.315	351.215	47.843	7.862
11	0.311	0.689	0.596	0.404	110.825	268.856	352.621	47.380	7.295
12	0.305	0.695	0.592	0.408	110.066	268.928	352.678	47.355	7.264
13	0.258	0.742	0.577	0.423	110.138	268.794	353.150	47.252	7.133
14	0.097	0.903	0.477	0.523	110.004	158.800	356.917	46.980	6.783

Table5.91 Simulation results using reflux ratio r = 1.55.

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.994	0.006	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.989	0.011	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.980	0.020	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.963	0.037	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.932	0.068	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.879	0.121	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.793	0.207	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.670	0.330	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.519	0.481	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.363	0.637	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.234	0.766	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.775	0.225	0.802	0.198	0.000	58.268	351.852	48.934	8.762
2	0.744	0.256	0.785	0.215	95.778	58.344	351.951	48.850	8.696
3	0.717	0.283	0.770	0.230	95.854	58.418	352.054	48.779	8.639
4	0.691	0.308	0.756	0.244	95.928	58.500	352.162	48.713	8.585
5	0.666	0.334	0.742	0.258	96.010	58.597	352.282	48.646	8.528
6	0.639	0.361	0.727	0.273	96.107	58.723	352.423	48.571	8.462
7	0.606	0.394	0.708	0.292	96.233	58.893	352.607	48.478	8.378
8	0.564	0.436	0.684	0.316	96.403	59.128	352.875	48.356	8.261
9	0.502	0.498	0.652	0.348	96.638	59.455	353.308	48.187	8.091
10	0.408	0.592	0.609	0.391	96.965	59.885	354.077	47.949	7.835
11	0.272	0.728	0.550	0.450	97.395	256.654	355.537	47.615	7.457
12	0.268	0.732	0.548	0.452	97.864	256.804	355.592	47.601	7.441
13	0.231	0.769	0.528	0.472	98.014	256.795	356.125	47.498	7.324
14	0.101	0.899	0.424	0.576	98.005	158.800	359.447	47.195	7.008

Table5.92 Simulation results at reflux ratio r=1.55 and %AAD of K-value = +9.25%.

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.993	0.007	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.988	0.012	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.979	0.021	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.961	0.039	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.930	0.070	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.875	0.124	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.789	0.211	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.666	0.334	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.516	0.484	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.362	0.638	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.234	0.766	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.799	0.201	0.831	0.169	0.000	58.268	352.290	49.149	8.888
2	0.761	0.239	0.803	0.197	95.778	58.392	352.460	49.028	8.796
3	0.725	0.275	0.779	0.221	95.902	58.516	352.637	48.920	8.710
4	0.691	0.309	0.755	0.245	96.026	58.648	352.826	48.816	8.624
5	0.656	0.344	0.731	0.269	96.158	58.794	353.043	48.709	8.532
6	0.616	0.384	0.706	0.294	96.304	58.956	353.305	48.592	8.428
7	0.569	0.431	0.677	0.323	96.466	59.136	353.642	48.460	8.305
8	0.512	0.488	0.646	0.354	96.646	59.335	354.094	48.311	8.159
9	0.442	0.558	0.611	0.389	96.845	59.562	354.717	48.139	7.984
10	0.357	0.643	0.572	0.428	97.072	59.833	355.591	47.938	7.771
11	0.259	0.741	0.524	0.476	97.343	257.084	356.860	47.697	7.511
12	0.249	0.751	0.518	0.482	98.294	257.143	357.011	47.666	7.478
13	0.206	0.794	0.493	0.507	98.353	257.107	357.733	47.557	7.362
14	0.091	0.909	0.389	0.611	98.317	158.800	361.104	47.268	7.099

Table5.93 Simulation results using reflux ratio r=1.55 and %AAD of K-value = -9.99%.

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.994	0.006	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.990	0.010	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.981	0.019	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.965	0.035	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.936	0.064	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.884	0.116	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.800	0.200	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.678	0.322	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.524	0.476	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.366	0.634	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.233	0.767	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.234	0.766	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.771	0.229	0.771	0.229	0.000	58.268	351.237	48.685	8.611
2	0.744	0.256	0.754	0.246	95.778	58.333	351.290	48.593	8.535
3	0.716	0.284	0.740	0.260	95.843	58.385	351.358	48.520	8.473
4	0.690	0.310	0.729	0.271	95.895	58.433	351.438	48.460	8.420
5	0.664	0.336	0.720	0.280	95.943	58.485	351.529	48.408	8.373
6	0.638	0.362	0.711	0.289	95.995	58.555	351.632	48.358	8.326
7	0.610	0.390	0.700	0.300	96.065	58.663	351.758	48.300	8.271
8	0.575	0.425	0.686	0.314	96.173	58.846	351.932	48.221	8.193
9	0.525	0.475	0.665	0.335	96.356	59.182	352.220	48.098	8.065
10	0.436	0.564	0.630	0.370	96.692	59.789	352.809	47.881	7.825
11	0.274	0.726	0.570	0.430	97.299	255.910	354.292	47.485	7.356
12	0.268	0.732	0.569	0.431	97.120	256.039	354.366	47.480	7.350
13	0.236	0.764	0.558	0.442	97.249	256.223	354.780	47.411	7.267
14	0.104	0.896	0.468	0.532	97.433	158.800	357.977	47.116	6.920

Table5.94 Simulation results using reflux ratio r=1.55 and %AAD of K-value = +22.77%.

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.993	0.006	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.988	0.012	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.979	0.021	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.961	0.039	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.930	0.070	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.876	0.124	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.790	0.210	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.667	0.333	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.516	0.484	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.362	0.638	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.234	0.766	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.795	0.205	0.841	0.159	0.000	58.268	353.131	49.326	8.961
2	0.723	0.277	0.790	0.210	95.778	58.450	353.681	49.137	8.810
3	0.658	0.342	0.745	0.255	95.960	58.617	354.227	48.968	8.668
4	0.596	0.404	0.704	0.296	96.127	58.769	354.784	48.812	8.533
5	0.537	0.463	0.667	0.333	96.279	58.905	355.358	48.667	8.403
6	0.481	0.519	0.634	0.366	96.415	59.025	355.952	48.531	8.279
7	0.427	0.573	0.604	0.396	96.535	59.136	356.558	48.405	8.161
8	0.378	0.622	0.577	0.423	96.646	59.252	357.172	48.286	8.049
9	0.331	0.669	0.550	0.450	96.762	59.391	357.797	48.170	7.939
10	0.286	0.714	0.521	0.479	96.901	59.571	358.464	48.045	7.819
11	0.241	0.759	0.487	0.513	97.081	257.808	359.233	47.897	7.679
12	0.230	0.770	0.481	0.519	99.018	257.934	359.424	47.871	7.655
13	0.193	0.807	0.453	0.547	99.144	258.044	360.161	47.758	7.550
14	0.098	0.902	0.355	0.645	99.254	158.800	362.943	47.441	7.296

Table5.95 Simulation results using reflux ratio r=1.55 and %AAD of K-value = -22.20%.

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.993	0.006	0.5	0.5	100.000	0.000	300.000	0.000	0.000
2	0.988	0.012	0.5	0.5	100.000	62.490	300.000	0.000	0.000
3	0.979	0.021	0.5	0.5	100.000	62.490	300.000	0.000	0.000
4	0.961	0.039	0.5	0.5	100.000	62.490	300.000	0.000	0.000
5	0.930	0.070	0.5	0.5	100.000	62.490	300.000	0.000	0.000
6	0.876	0.124	0.5	0.5	100.000	62.490	300.000	0.000	0.000
7	0.790	0.210	0.5	0.5	100.000	62.490	300.000	0.000	0.000
8	0.667	0.333	0.5	0.5	100.000	62.490	300.000	0.000	0.000
9	0.516	0.484	0.5	0.5	100.000	62.490	300.000	0.000	0.000
10	0.362	0.638	0.5	0.5	100.000	62.490	300.000	0.000	0.000
11	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
12	0.232	0.768	0.5	0.5	100.000	258.790	300.000	0.000	0.000
13	0.234	0.766	0.5	0.5	100.000	258.790	300.000	0.000	0.000
14	0.229	0.771	0.5	0.5	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.795	0.205	0.841	0.159	0.000	58.268	353.131	49.326	8.961
2	0.723	0.277	0.790	0.210	95.778	58.450	353.681	49.137	8.810
3	0.658	0.342	0.745	0.255	95.960	58.617	354.227	48.968	8.668
4	0.596	0.404	0.704	0.296	96.127	58.769	354.784	48.812	8.533
5	0.537	0.463	0.667	0.333	96.279	58.905	355.358	48.667	8.403
6	0.481	0.519	0.634	0.366	96.415	59.025	355.952	48.531	8.279
7	0.427	0.573	0.604	0.396	96.535	59.136	356.558	48.405	8.161
8	0.378	0.622	0.577	0.423	96.646	59.252	357.172	48.286	8.049
9	0.331	0.669	0.550	0.450	96.762	59.391	357.797	48.170	7.939
10	0.286	0.714	0.521	0.479	96.901	59.571	358.464	48.045	7.819
11	0.241	0.759	0.487	0.513	97.081	257.808	359.233	47.897	7.679
12	0.230	0.770	0.481	0.519	99.018	257.934	359.424	47.871	7.655
13	0.193	0.807	0.453	0.547	99.144	258.044	360.161	47.758	7.550
14	0.098	0.902	0.355	0.645	99.254	158.800	362.943	47.441	7.296

Table5.96 %AAD of composition (x_1) profile by varying reflux ratio at K-value=+9.25%.

Stage	$X_{1r=1.55}$	$X_{1r=1.55(+9.25\%)}$	Δ	$X_{1r=1.9}$	$X_{1r=1.9(+9.25\%)}$	Δ	$X_{1r=1.7}$	$X_{1r=1.7(+9.25\%)}$	Δ
1	0.775	0.799	0.0310	0.793	0.814	0.0265	0.786	0.807	0.0267
2	0.744	0.761	0.0228	0.763	0.783	0.0262	0.755	0.773	0.0238
3	0.717	0.725	0.0112	0.735	0.754	0.0259	0.725	0.741	0.0221
4	0.691	0.691	0.0000	0.706	0.724	0.0255	0.696	0.709	0.0187
5	0.666	0.656	0.0150	0.677	0.693	0.0236	0.667	0.676	0.0135
6	0.639	0.616	0.0360	0.646	0.658	0.0186	0.637	0.639	0.0031
7	0.606	0.569	0.0611	0.611	0.616	0.0082	0.602	0.595	0.0116
8	0.564	0.512	0.0922	0.569	0.562	0.0123	0.56	0.539	0.0375
9	0.502	0.442	0.1195	0.511	0.490	0.0411	0.502	0.468	0.0677
10	0.408	0.357	0.1250	0.423	0.395	0.0662	0.413	0.377	0.0872
11	0.272	0.259	0.0478	0.279	0.273	0.0215	0.274	0.266	0.0292
12	0.268	0.249	0.0709	0.273	0.260	0.0476	0.268	0.254	0.0522
13	0.231	0.206	0.1082	0.235	0.209	0.1106	0.231	0.208	0.0996
14	0.101	0.091	0.0990	0.100	0.086	0.1400	0.101	0.089	0.1188
Sum of data			0.8397			0.5938			0.6118

N = number of data points

$$\Delta = \left| \frac{x_{1at\ \%AAD} - x_{1accurate}}{x_{1accurate}} \right|$$

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N} \left| \frac{x_{1at\ \%AAD} - x_{1accurate}}{x_{1accurate}} \right| \right] x100$$

At r=1.55 and +9.25%AAD of K-value = (0.8397x100)/14

= 6.00%

At r=1.9 and +9.25%AAD of K-value = (0.5938x100)/14

= 4.24%

At r=1.7 and +9.25%AAD of K-value = (0.6118x100)/14

= 4.37%

Table5.97 %AAD of composition (x_1) profile by varying reflux ratio at K-value=+22.77%.

Stage	$X_{1r=1.55}$	$X_{1r=1.55(+22.77\%)}$	Δ	$X_{1r=1.9}$	$X_{1r=1.9(+22.77\%)}$	Δ	$X_{1r=1.7}$	$X_{1r=1.7(+22.77\%)}$	Δ
1	0.775	0.795	0.0258	0.793	0.826	0.0390	0.786	0.812	0.0331
2	0.744	0.723	0.0282	0.763	0.768	0.0622	0.755	0.748	0.0093
3	0.717	0.658	0.0823	0.735	0.713	0.0836	0.725	0.688	0.0510
4	0.691	0.596	0.1375	0.706	0.659	0.1057	0.696	0.630	0.0948
5	0.666	0.537	0.1937	0.677	0.604	0.1248	0.667	0.574	0.1394
6	0.639	0.481	0.2473	0.646	0.549	0.1414	0.637	0.517	0.1884
7	0.606	0.427	0.2954	0.611	0.492	0.1522	0.602	0.462	0.2326
8	0.564	0.378	0.3298	0.569	0.434	0.1481	0.560	0.407	0.2732
9	0.502	0.331	0.3406	0.511	0.375	0.1329	0.502	0.353	0.2968
10	0.408	0.286	0.2990	0.423	0.314	0.0979	0.413	0.300	0.2736
11	0.272	0.241	0.1140	0.279	0.249	0.0332	0.274	0.245	0.1058
12	0.268	0.230	0.1418	0.273	0.236	0.0261	0.268	0.233	0.1306
13	0.231	0.193	0.1645	0.235	0.193	0.0000	0.231	0.193	0.1645
14	0.101	0.098	0.0297	0.100	0.091	0.0714	0.101	0.094	0.0693
Sum of data			2.4295			1.2186			2.0625

N = number of data points

$$\Delta = \left| \frac{x_{1\text{at }\%AAD} - x_{1accurate}}{x_{1accurate}} \right|$$

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\frac{x_{1\text{at }\%AAD} - x_{1accurate}}{x_{1accurate}}\right|\right] x100$$

At r=1.55 and +22.77%AAD of K-value = (2.4295x100)/14

= 17.35%

At r=1.9 and +22.77%AAD of K-value = (1.2186x100)/14

= 8.70%

At r=1.7 and +22.77%AAD of K-value = (2.0625x100)/14

= 14.73%

Table5.98 %AAD of composition (x_1) profile by varying reflux ratio at K-value= -9.99%.

Stage	$X_{1r=1.55}$	$X_{1r=1.55(-9.99\%)}$	Δ	$X_{1r=1.9}$	$X_{1r=1.9(-9.99\%)}$	Δ	$X_{1r=1.7}$	$X_{1r=1.7(-9.99\%)}$	Δ
1	0.775	0.771	0.0052	0.793	0.770	0.0290	0.786	0.785	0.0013
2	0.744	0.744	0.0000	0.763	0.748	0.0197	0.755	0.777	0.0291
3	0.717	0.716	0.0014	0.735	0.728	0.0095	0.725	0.765	0.0552
4	0.691	0.690	0.0014	0.706	0.708	0.0028	0.696	0.749	0.0761
5	0.666	0.664	0.0030	0.677	0.689	0.0177	0.667	0.729	0.0930
6	0.639	0.638	0.0016	0.646	0.668	0.0341	0.637	0.702	0.1020
7	0.606	0.610	0.0066	0.611	0.643	0.0524	0.602	0.668	0.1096
8	0.564	0.575	0.0195	0.569	0.609	0.0703	0.56	0.622	0.1107
9	0.502	0.525	0.0458	0.511	0.558	0.0920	0.502	0.559	0.1135
10	0.408	0.436	0.0686	0.423	0.468	0.1064	0.413	0.459	0.1114
11	0.272	0.274	0.0074	0.279	0.292	0.0466	0.274	0.286	0.0438
12	0.268	0.268	0.0000	0.273	0.288	0.0549	0.268	0.277	0.0336
13	0.231	0.236	0.0216	0.235	0.252	0.0723	0.231	0.233	0.0087
14	0.101	0.104	0.0297	0.100	0.105	0.0500	0.101	0.093	0.0792
Sum of data			0.2118			0.6577			0.9672

N = number of data points

$$\Delta = \left| \frac{x_{1at\ \%AAD} - x_{1accurate}}{x_{1accurate}} \right|$$

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\frac{x_{1at\ \%AAD} - x_{1accurate}}{x_{1accurate}}\right|\right]x100$$

At r=1.55 and –9.99%AAD of K-value = (0.2118x100)/14

= 1.51%

At r=1.9 and –9.99%AAD of K-value = (0.6577x100)/14

= 4.70%

At r=1.7 and –9.99%AAD of K-value = (0.9672x100)/14

= 6.91%

Table5.99 %AAD of composition (x_1) profile by varying reflux ratio at K-value= -22.20%.

Stage	$X_{1r=1.55}$	$X_{1r=1.55(-22.20\%)}$	Δ	$X_{1r=1.9}$	$X_{1r=1.9(-22.20\%)}$	Δ	$X_{1r=1.7}$	$X_{1r=1.7(-22.20\%)}$	Δ
1	0.775	0.795	0.0258	0.793	0.765	0.0353	0.786	0.724	0.0789
2	0.744	0.723	0.0282	0.763	0.775	0.0157	0.755	0.715	0.0530
3	0.717	0.658	0.0823	0.735	0.779	0.0599	0.725	0.712	0.0179
4	0.691	0.596	0.1375	0.706	0.776	0.0992	0.696	0.712	0.0230
5	0.666	0.537	0.1937	0.677	0.765	0.1300	0.667	0.711	0.0660
6	0.639	0.481	0.2473	0.646	0.746	0.1548	0.637	0.706	0.1083
7	0.606	0.427	0.2954	0.611	0.719	0.1768	0.602	0.692	0.1495
8	0.564	0.378	0.3298	0.569	0.681	0.1968	0.56	0.666	0.1893
9	0.502	0.331	0.3406	0.511	0.624	0.2211	0.502	0.617	0.2291
10	0.408	0.286	0.2990	0.423	0.525	0.2411	0.413	0.519	0.2567
11	0.272	0.241	0.1140	0.279	0.311	0.1147	0.274	0.303	0.1058
12	0.268	0.230	0.1418	0.273	0.305	0.1172	0.268	0.304	0.1343
13	0.231	0.193	0.1645	0.235	0.258	0.0979	0.231	0.274	0.1861
14	0.101	0.098	0.0297	0.100	0.097	0.0300	0.101	0.113	0.1188
Sum of data			2.4295			1.6905			1.7167

N = number of data points

$$\Delta = \left|\frac{x_{1at\ \%AAD} - x_{1accurate}}{x_{1accurate}}\right|$$

%Average Absolute Deviation = $\frac{1}{N}\left[\sum_{N}\left|\frac{x_{1at\ \%AAD} - x_{1accurate}}{x_{1accurate}}\right|\right]$x100

At r=1.55 and –22.20%AAD of K-value = (2.4295x100)/14

= 17.35%

At r=1.9 and –22.20%AAD of K-value = (1.6905x100)/14

= 12.08%

At r=1.7 and –22.20%AAD of K-value = (1.7167x100)/14

= 12.26%

Table5.100 %AAD of temperature profile by varying reflux ratio at K-value = +9.25%.

Stage	$T_{r=1.55}$	$T_{r=1.55(+9.25\%)}$	Δ	$T_{r=1.9}$	$T_{r=1.9(+9.25\%)}$	Δ	$T_{r=1.7}$	$T_{r=1.7(+9.25\%)}$	Δ
1	351.852	352.290	0.0012	351.811	352.227	0.0012	351.827	352.255	0.0012
2	351.951	352.460	0.0014	351.895	352.357	0.0013	351.921	352.403	0.0014
3	352.054	352.637	0.0017	351.993	352.493	0.0014	352.028	352.557	0.0015
4	352.162	352.826	0.0019	352.106	352.643	0.0015	352.147	352.724	0.0016
5	352.282	353.043	0.0022	352.236	352.816	0.0016	352.282	352.915	0.0018
6	352.423	353.305	0.0025	352.391	353.029	0.0018	352.439	353.149	0.0020
7	352.607	353.642	0.0029	352.583	353.308	0.0021	352.634	353.454	0.0023
8	352.875	354.094	0.0035	352.842	353.699	0.0024	352.898	353.873	0.0028
9	353.308	354.717	0.0040	353.236	354.280	0.0030	353.304	354.476	0.0033
10	354.077	355.591	0.0043	353.941	355.182	0.0035	354.027	355.372	0.0038
11	355.537	356.860	0.0037	355.437	356.648	0.0034	355.505	356.752	0.0035
12	355.592	357.011	0.0040	355.516	356.838	0.0037	355.582	356.923	0.0038
13	356.125	357.733	0.0045	356.057	357.675	0.0045	356.11	357.704	0.0045
14	359.447	361.104	0.0046	359.466	361.361	0.0053	359.443	361.239	0.0050
Sum of data			0.0424			0.0368			0.0385

N = number of data points

$$\Delta = \left| \frac{T_{\text{at \%AAD}} - T_{\text{accurate}}}{T_{\text{accurate}}} \right|$$

%Average Absolute Deviation = $\frac{1}{N}\left[\sum_{N} \left| \frac{T_{\text{at \%AAD}} - T_{\text{accurate}}}{T_{\text{accurate}}} \right|\right]$x100

At r=1.55 and +9.25%AAD of K-value = (0.0424x100)/14

= 0.30%

At r=1.9 and +9.25%AAD of K-value = (0.0368x100)/14

= 0.26%

At r=1.7 and +9.25%AAD of K-value = (0.0385x100)/14

= 0.28%

Table5.101 %AAD of temperature profile by varying reflux ratio at K-value=+22.77%.

Stage	$T_{r=1.55}$	$T_{r=1.55(+22.77\%)}$	Δ	$T_{r=1.9}$	$T_{r=1.9(+22.77\%)}$	Δ	$T_{r=1.7}$	$T_{r=1.7(+22.77\%)}$	Δ
1	351.852	353.131	0.0036	351.811	352.911	0.0031	351.827	353.009	0.0034
2	351.951	353.681	0.0049	351.895	353.333	0.0041	351.921	353.487	0.0044
3	352.054	354.227	0.0062	351.993	353.764	0.0050	352.028	353.968	0.0055
4	352.162	354.784	0.0074	352.106	354.217	0.0060	352.147	354.467	0.0066
5	352.282	355.358	0.0087	352.236	354.704	0.0070	352.282	354.995	0.0077
6	352.423	355.952	0.0100	352.391	355.237	0.0081	352.439	355.559	0.0089
7	352.607	356.558	0.0112	352.583	355.826	0.0092	352.634	356.162	0.0100
8	352.875	357.172	0.0122	352.842	356.480	0.0103	352.898	356.805	0.0111
9	353.308	357.797	0.0127	353.236	357.210	0.0113	353.304	357.493	0.0119
10	354.077	358.464	0.0124	353.941	358.051	0.0116	354.027	358.256	0.0119
11	355.537	359.233	0.0104	355.437	359.080	0.0102	355.505	359.161	0.0103
12	355.592	359.424	0.0108	355.516	359.306	0.0107	355.582	359.371	0.0107
13	356.125	360.161	0.0113	356.057	360.166	0.0115	356.11	360.171	0.0114
14	359.447	362.943	0.0097	359.466	363.246	0.0105	359.443	363.108	0.0102
Sum of data			0.1316			0.1187			0.1239

N = number of data points

$$\Delta = \left|\frac{T_{at\ \%AAD} - T_{accurate}}{T_{accurate}}\right|$$

%Average Absolute Deviation = $\frac{1}{N}\left[\sum_{N}\left|\frac{T_{at\ \%AAD} - T_{accurate}}{T_{accurate}}\right|\right]x100$

At r=1.55 and +22.77%AAD of K-value = (0.1316x100)/14

= 0.94%

At r=1.9 and +22.77%AAD of K-value = (0.1187x100)/14

= 0.85%

At r=1.7 and +22.77%AAD of K-value = (0.1239x100)/14

= 0.89%

Table5.102 %AAD of temperature profile by varying reflux ratio at K-value= -9.99%.

Stage	$T_{r=1.55}$	$T_{r=1.55(-9.99\%)}$	Δ	$T_{r=1.9}$	$T_{r=1.9(-9.99\%)}$	Δ	$T_{r=1.7}$	$T_{r=1.7(-9.99\%)}$	Δ
1	351.852	351.237	0.0017	351.811	351.236	0.0016	351.827	351.205	0.0018
2	351.951	351.290	0.0019	351.895	351.274	0.0018	351.921	351.220	0.0020
3	352.054	351.358	0.0020	351.993	351.320	0.0019	352.028	351.242	0.0022
4	352.162	351.438	0.0021	352.106	351.372	0.0021	352.147	351.275	0.0025
5	352.282	351.529	0.0021	352.236	351.433	0.0023	352.282	351.325	0.0027
6	352.423	351.632	0.0022	352.391	351.508	0.0025	352.439	351.402	0.0029
7	352.607	351.758	0.0024	352.583	351.607	0.0028	352.634	351.521	0.0032
8	352.875	351.932	0.0027	352.842	351.759	0.0031	352.898	351.711	0.0034
9	353.308	352.220	0.0031	353.236	352.025	0.0034	353.304	352.032	0.0036
10	354.077	352.809	0.0036	353.941	352.587	0.0038	354.027	352.652	0.0039
11	355.537	354.292	0.0035	355.437	354.089	0.0038	355.505	354.152	0.0038
12	355.592	354.366	0.0034	355.516	354.135	0.0039	355.582	354.256	0.0037
13	356.125	354.780	0.0038	356.057	354.564	0.0042	356.110	354.824	0.0036
14	359.447	357.977	0.0041	359.466	357.943	0.0042	359.443	358.488	0.0027
Sum of data			0.0386			0.0414			0.0419

N = number of data points

$$\Delta = \left| \frac{T_{\text{at \%AAD}} - T_{\text{accurate}}}{T_{\text{accurate}}} \right|$$

$$\text{\%Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\frac{T_{\text{at \%AAD}} - T_{\text{accurate}}}{T_{\text{accurate}}}\right|\right]\text{x}100$$

At r=1.55 and –9.99%AAD of K-value = (0.0386x100)/14

= 0.28%

At r=1.9 and –9.99%AAD of K-value = (0.0414x100)/14

= 0.30%

At r=1.7 and –9.99%AAD of K-value = (0.0419x100)/14

= 0.30%

Table5.103 %AAD of temperature profile by varying reflux ratio at K-value= -22.20%.

Stage	$T_{r=1.55}$	$T_{r=1.55(-22.20\%)}$	Δ	$T_{r=1.9}$	$T_{r=1.9(-22.20\%)}$	Δ	$T_{r=1.7}$	$T_{r=1.7(-22.20\%)}$	Δ
1	351.852	353.131	0.0036	351.811	350.471	0.0038	351.827	350.517	0.0037
2	351.951	353.681	0.0049	351.895	350.472	0.0040	351.921	350.526	0.0040
3	352.054	354.227	0.0062	351.993	350.477	0.0043	352.028	350.527	0.0043
4	352.162	354.784	0.0074	352.106	350.482	0.0046	352.147	350.526	0.0046
5	352.282	355.358	0.0087	352.236	350.488	0.0050	352.282	350.528	0.0050
6	352.423	355.952	0.0100	352.391	350.504	0.0054	352.439	350.541	0.0054
7	352.607	356.558	0.0112	352.583	350.540	0.0058	352.634	350.572	0.0058
8	352.875	357.172	0.0122	352.842	350.620	0.0063	352.898	350.643	0.0064
9	353.308	357.797	0.0127	353.236	350.792	0.0069	353.304	350.807	0.0071
10	354.077	358.464	0.0124	353.941	351.215	0.0077	354.027	351.239	0.0079
11	355.537	359.233	0.0104	355.437	352.621	0.0079	355.505	352.691	0.0079
12	355.592	359.424	0.0108	355.516	352.678	0.0080	355.582	352.681	0.0082
13	356.125	360.161	0.0113	356.057	353.150	0.0082	356.110	352.978	0.0088
14	359.447	362.943	0.0097	359.466	356.917	0.0071	359.443	356.173	0.0091
Sum of data			0.1316			0.0850			0.0881

N = number of data points

$$\Delta = \left| \frac{T_{at\ \%AAD} - T_{accurate}}{T_{accurate}} \right|$$

%Average Absolute Deviation = $\frac{1}{N}\left[\sum_{N} \left| \frac{T_{at\ \%AAD} - T_{accurate}}{T_{accurate}} \right| \right]$x100

At r=1.55 and –22.20%AAD of K-value = (0.1316x100)/14

= 0.94%

At r=1.9 and –22.20%AAD of K-value = (0.0850x100)/14

= 0.61%

At r=1.7 and –22.20%AAD of K-value = (0.0881x100)/14

= 0.63%

Table5.104 Simulation results using number of stage N=10.

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.959	0.041	0.500	0.500	100.000	0.000	300.000	0.000	0.000
2	0.929	0.071	0.500	0.500	100.000	62.490	300.000	0.000	0.000
3	0.878	0.122	0.500	0.500	100.000	62.490	300.000	0.000	0.000
4	0.793	0.207	0.500	0.500	100.000	62.490	300.000	0.000	0.000
5	0.670	0.330	0.500	0.500	100.000	62.490	300.000	0.000	0.000
6	0.519	0.481	0.500	0.500	100.000	62.490	300.000	0.000	0.000
7	0.364	0.636	0.500	0.500	100.000	62.490	300.000	0.000	0.000
8	0.232	0.768	0.500	0.500	100.000	258.790	300.000	0.000	0.000
9	0.234	0.766	0.500	0.500	100.000	258.790	300.000	0.000	0.000
10	0.229	0.771	0.500	0.500	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.773	0.227	0.789	0.211	0.000	64.742	351.867	48.874	8.715
2	0.731	0.269	0.760	0.240	102.252	64.897	352.012	48.733	8.602
3	0.685	0.315	0.733	0.267	102.407	65.046	352.203	48.601	8.489
4	0.635	0.365	0.707	0.293	102.556	65.198	352.457	48.471	8.371
5	0.576	0.424	0.681	0.319	102.708	65.379	352.799	48.338	8.244
6	0.506	0.494	0.652	0.348	102.889	65.671	353.280	48.187	8.091
7	0.411	0.589	0.614	0.386	103.181	66.224	354.048	47.976	7.865
8	0.267	0.733	0.551	0.449	103.734	263.101	355.597	47.619	7.461
9	0.231	0.769	0.535	0.465	104.311	263.290	356.113	47.535	7.365
10	0.104	0.896	0.439	0.561	104.500	158.800	359.318	47.219	7.027

Table5.105 Simulation resultsusingt N=10 and %AAD of K-value = +9.25%.

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.958	0.042	0.500	0.500	100.000	0.000	300.000	0.000	0.000
2	0.927	0.073	0.500	0.500	100.000	62.490	300.000	0.000	0.000
3	0.875	0.125	0.500	0.500	100.000	62.490	300.000	0.000	0.000
4	0.789	0.211	0.500	0.500	100.000	62.490	300.000	0.000	0.000
5	0.666	0.334	0.500	0.500	100.000	62.490	300.000	0.000	0.000
6	0.516	0.484	0.500	0.500	100.000	62.490	300.000	0.000	0.000
7	0.362	0.638	0.500	0.500	100.000	62.490	300.000	0.000	0.000
8	0.232	0.768	0.500	0.500	100.000	258.790	300.000	0.000	0.000
9	0.234	0.766	0.500	0.500	100.000	258.790	300.000	0.000	0.000
10	0.229	0.771	0.500	0.500	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.773	0.227	0.806	0.194	0.000	64.742	352.409	49.040	8.805
2	0.719	0.281	0.771	0.229	102.252	64.909	352.674	48.884	8.680
3	0.665	0.335	0.739	0.261	102.419	65.070	352.982	48.739	8.559
4	0.609	0.391	0.708	0.292	102.580	65.237	353.348	48.599	8.435
5	0.548	0.452	0.677	0.323	102.747	65.440	353.800	48.455	8.301
6	0.477	0.523	0.643	0.357	102.950	65.751	354.390	48.291	8.140
7	0.387	0.613	0.598	0.402	103.261	66.234	355.265	48.068	7.910
8	0.263	0.737	0.532	0.468	103.744	263.705	356.787	47.736	7.553
9	0.225	0.775	0.509	0.491	104.915	263.786	357.392	47.625	7.435
10	0.103	0.897	0.405	0.595	104.996	158.800	360.556	47.297	7.118

Table5.106 Simulation results using N=10 and %AAD of K-value = -9.99%.

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.962	0.038	0.500	0.500	100.000	0.000	300.000	0.000	0.000
2	0.933	0.067	0.500	0.500	100.000	62.490	300.000	0.000	0.000
3	0.883	0.117	0.500	0.500	100.000	62.490	300.000	0.000	0.000
4	0.800	0.200	0.500	0.500	100.000	62.490	300.000	0.000	0.000
5	0.678	0.322	0.500	0.500	100.000	62.490	300.000	0.000	0.000
6	0.524	0.476	0.500	0.500	100.000	62.490	300.000	0.000	0.000
7	0.366	0.634	0.500	0.500	100.000	62.490	300.000	0.000	0.000
8	0.233	0.767	0.500	0.500	100.000	258.790	300.000	0.000	0.000
9	0.234	0.766	0.500	0.500	100.000	258.790	300.000	0.000	0.000
10	0.229	0.771	0.500	0.500	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.770	0.230	0.787	0.213	0.000	64.742	351.227	48.770	8.678
2	0.752	0.248	0.772	0.228	102.252	64.900	351.262	48.689	8.614
3	0.729	0.271	0.752	0.248	102.410	65.088	351.320	48.587	8.531
4	0.696	0.304	0.729	0.271	102.598	65.302	351.419	48.461	8.421
5	0.648	0.352	0.701	0.299	102.812	65.550	351.599	48.308	8.279
6	0.576	0.424	0.669	0.331	103.060	65.883	351.938	48.122	8.091
7	0.464	0.536	0.629	0.371	103.393	66.482	352.619	47.874	7.817
8	0.279	0.721	0.568	0.432	103.992	262.641	354.232	47.470	7.337
9	0.237	0.763	0.551	0.449	103.851	262.631	354.771	47.378	7.226
10	0.097	0.903	0.456	0.544	103.841	158.800	358.296	47.100	6.904

Table5.107 Simulation results using N=10 and %AAD of K-value = +22.77%.

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.958	0.042	0.500	0.500	100.000	0.000	300.000	0.000	0.000
2	0.927	0.073	0.500	0.500	100.000	62.490	300.000	0.000	0.000
3	0.875	0.125	0.500	0.500	100.000	62.490	300.000	0.000	0.000
4	0.790	0.210	0.500	0.500	100.000	62.490	300.000	0.000	0.000
5	0.667	0.333	0.500	0.500	100.000	62.490	300.000	0.000	0.000
6	0.516	0.484	0.500	0.500	100.000	62.490	300.000	0.000	0.000
7	0.362	0.638	0.500	0.500	100.000	62.490	300.000	0.000	0.000
8	0.232	0.768	0.500	0.500	100.000	258.790	300.000	0.000	0.000
9	0.234	0.766	0.500	0.500	100.000	258.790	300.000	0.000	0.000
10	0.229	0.771	0.500	0.500	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.776	0.224	0.831	0.169	0.000	64.742	353.268	49.288	8.932
2	0.696	0.304	0.775	0.225	102.252	64.962	353.896	49.082	8.764
3	0.620	0.380	0.724	0.276	102.472	65.164	354.558	48.889	8.600
4	0.545	0.455	0.678	0.322	102.674	65.357	355.272	48.707	8.439
5	0.472	0.528	0.634	0.366	102.867	65.562	356.050	48.529	8.277
6	0.398	0.602	0.590	0.410	103.072	65.814	356.916	48.346	8.106
7	0.322	0.678	0.543	0.457	103.324	66.120	357.926	48.140	7.909
8	0.244	0.756	0.486	0.514	103.630	264.474	359.179	47.896	7.678
9	0.202	0.798	0.453	0.547	105.684	264.498	359.973	47.760	7.552
10	0.101	0.899	0.353	0.647	105.708	158.800	362.840	47.437	7.293

Table5.108 Simulation results using N=10 and %AAD of K-value = -22.20%.

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.966	0.034	0.500	0.500	100.000	0.000	300.000	0.000	0.000
2	0.939	0.061	0.500	0.500	100.000	62.490	300.000	0.000	0.000
3	0.892	0.108	0.500	0.500	100.000	62.490	300.000	0.000	0.000
4	0.812	0.188	0.500	0.500	100.000	62.490	300.000	0.000	0.000
5	0.690	0.310	0.500	0.500	100.000	62.490	300.000	0.000	0.000
6	0.534	0.466	0.500	0.500	100.000	62.490	300.000	0.000	0.000
7	0.371	0.629	0.500	0.500	100.000	62.490	300.000	0.000	0.000
8	0.233	0.767	0.500	0.500	100.000	258.790	300.000	0.000	0.000
9	0.235	0.765	0.500	0.500	100.000	258.790	300.000	0.000	0.000
10	0.229	0.771	0.500	0.500	100.000	158.800	300.000	0.000	0.000

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.724	0.276	0.739	0.261	0.000	64.742	350.523	48.390	8.421
2	0.699	0.301	0.735	0.265	102.252	64.748	350.563	48.362	8.396
3	0.680	0.320	0.732	0.268	102.258	64.788	350.604	48.344	8.381
4	0.662	0.338	0.728	0.272	102.298	64.890	350.650	48.318	8.357
5	0.640	0.360	0.718	0.282	102.400	65.103	350.718	48.264	8.307
6	0.601	0.399	0.700	0.300	102.613	65.530	350.862	48.149	8.195
7	0.514	0.486	0.664	0.335	103.040	66.458	351.258	47.913	7.942
8	0.300	0.700	0.598	0.402	103.968	262.233	352.715	47.397	7.316
9	0.271	0.729	0.587	0.413	103.443	262.423	353.001	47.319	7.218
10	0.115	0.885	0.499	0.501	103.633	158.800	356.112	46.998	6.804

Table5.109 Simulation results using number of stage N =20.

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	1	0	0.5	0.5	100.000	0	300.000	0.000	0.000
2	0.999	0.001	0.5	0.5	100.000	62.49	300.000	0.000	0.000
3	0.998	0.002	0.5	0.5	100.000	62.49	300.000	0.000	0.000
4	0.997	0.003	0.5	0.5	100.000	62.49	300.000	0.000	0.000
5	0.994	0.006	0.5	0.5	100.000	62.49	300.000	0.000	0.000
6	0.989	0.011	0.5	0.5	100.000	62.49	300.000	0.000	0.000
7	0.980	0.020	0.5	0.5	100.000	62.49	300.000	0.000	0.000
8	0.963	0.037	0.5	0.5	100.000	62.49	300.000	0.000	0.000
9	0.932	0.068	0.5	0.5	100.000	62.49	300.000	0.000	0.000
10	0.879	0.121	0.5	0.5	100.000	62.49	300.000	0.000	0.000
11	0.793	0.207	0.5	0.5	100.000	62.49	300.000	0.000	0.000
12	0.670	0.330	0.5	0.5	100.000	62.49	300.000	0.000	0.000
13	0.519	0.481	0.5	0.5	100.000	62.49	300.000	0.000	0.000
14	0.363	0.637	0.5	0.5	100.000	62.49	300.000	0.000	0.000
15	0.232	0.768	0.5	0.5	100.000	258.79	300.000	0.000	0.000
16	0.232	0.768	0.5	0.5	100.000	258.79	300.000	0.000	0.000
17	0.232	0.768	0.5	0.5	100.000	258.79	300.000	0.000	0.000
18	0.232	0.768	0.5	0.5	100.000	258.79	300.000	0.000	0.000
19	0.234	0.766	0.5	0.5	100.000	258.79	300.000	0.000	0.000
20	0.229	0.771	0.5	0.5	100.000	158.80	300.000	0.000	0.000

Table5.109 (continued)

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.800	0.200	0.816	0.184	0	64.746	351.786	49.044	8.814
2	0.779	0.221	0.804	0.196	102.252	64.806	351.84	48.943	8.768
3	0.761	0.239	0.793	0.207	102.316	64.869	351.896	48.89	8.727
4	0.743	0.257	0.782	0.218	102.379	64.934	351.955	48.839	8.687
5	0.727	0.273	0.771	0.229	102.444	65.002	352.018	48.788	8.646
6	0.709	0.291	0.760	0.240	102.512	65.075	352.088	48.735	8.603
7	0.691	0.309	0.749	0.251	102.585	65.153	352.169	48.68	8.557
8	0.670	0.330	0.737	0.263	102.663	65.239	352.266	48.619	8.505
9	0.647	0.353	0.723	0.277	102.749	65.333	352.386	48.553	8.446
10	0.619	0.381	0.708	0.292	102.843	65.443	352.538	48.479	8.379
11	0.585	0.415	0.691	0.309	102.953	65.580	352.739	48.393	8.298
12	0.542	0.458	0.671	0.329	103.09	65.768	353.019	48.289	8.195
13	0.484	0.516	0.645	0.355	103.278	66.061	353.442	48.151	8.053
14	0.399	0.601	0.609	0.391	103.571	66.527	354.158	47.947	7.833
15	0.270	0.730	0.553	0.447	104.037	263.264	355.559	47.628	7.471
16	0.270	0.730	0.555	0.445	104.474	263.336	355.556	47.641	7.486
17	0.272	0.728	0.557	0.443	104.546	263.453	355.527	47.651	7.498
18	0.270	0.730	0.554	0.446	104.663	263.647	355.557	47.636	7.481
19	0.232	0.768	0.531	0.469	104.857	263.605	356.099	47.518	7.345
20	0.099	0.901	0.423	0.577	104.815	158.80	359.551	47.194	7.007

Table5.110 Simulation results using N =20 and %AAD of K-value = +9.25%.

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.999	0.000	0.5	0.5	100.000	0	300.000	0.000	0.000
2	0.999	0.000	0.5	0.5	100.000	62.49	300.000	0.000	0.000
3	0.998	0.002	0.5	0.5	100.000	62.49	300.000	0.000	0.000
4	0.997	0.003	0.5	0.5	100.000	62.49	300.000	0.000	0.000
5	0.994	0.006	0.5	0.5	100.000	62.49	300.000	0.000	0.000
6	0.989	0.011	0.5	0.5	100.000	62.49	300.000	0.000	0.000
7	0.979	0.021	0.5	0.5	100.000	62.49	300.000	0.000	0.000
8	0.961	0.039	0.5	0.5	100.000	62.49	300.000	0.000	0.000
9	0.930	0.070	0.5	0.5	100.000	62.49	300.000	0.000	0.000
10	0.876	0.124	0.5	0.5	100.000	62.49	300.000	0.000	0.000
11	0.789	0.211	0.5	0.5	100.000	62.49	300.000	0.000	0.000
12	0.666	0.334	0.5	0.5	100.000	62.49	300.000	0.000	0.000
13	0.516	0.484	0.5	0.5	100.000	62.49	300.000	0.000	0.000
14	0.362	0.638	0.5	0.5	100.000	62.49	300.000	0.000	0.000
15	0.232	0.768	0.5	0.5	100.000	258.79	300.000	0.000	0.000
16	0.232	0.768	0.5	0.5	100.000	258.79	300.000	0.000	0.000
17	0.232	0.768	0.5	0.5	100.000	258.79	300.000	0.000	0.000
18	0.232	0.768	0.5	0.5	100.000	258.79	300.000	0.000	0.000
19	0.234	0.766	0.5	0.5	100.000	258.79	300.000	0.000	0.000
20	0.229	0.771	0.5	0.5	100.000	158.80	300.000	0.000	0.000

Table5.110 (continued)

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.826	0.174	0.849	0.151	0.000	64.742	352.184	49.230	8.947
2	0.798	0.202	0.827	0.173	102.252	64.846	352.297	49.131	8.874
3	0.772	0.228	0.807	0.193	102.356	64.942	352.410	49.044	8.808
4	0.748	0.252	0.789	0.211	102.452	65.032	352.526	48.965	8.746
5	0.724	0.276	0.772	0.228	102.542	65.120	352.649	48.890	8.685
6	0.700	0.300	0.756	0.244	102.630	65.205	352.782	48.817	8.625
7	0.675	0.325	0.740	0.260	102.715	65.291	352.928	48.745	8.564
8	0.648	0.352	0.724	0.276	102.801	65.381	353.094	48.673	8.501
9	0.619	0.381	0.707	0.293	102.891	65.479	353.286	48.598	8.433
10	0.586	0.414	0.690	0.310	102.989	65.592	353.514	48.517	8.359
11	0.549	0.451	0.670	0.330	103.102	65.734	353.796	48.425	8.271
12	0.503	0.497	0.647	0.353	103.244	65.924	354.166	48.315	8.163
13	0.445	0.555	0.618	0.382	103.434	66.187	354.684	48.172	8.018
14	0.368	0.632	0.580	0.420	103.697	66.518	355.472	47.978	7.814
15	0.267	0.733	0.529	0.471	104.028	263.772	356.730	47.721	7.537
16	0.268	0.732	0.527	0.473	104.982	263.757	356.721	47.712	7.528
17	0.265	0.735	0.524	0.476	104.967	263.730	356.769	47.695	7.510
18	0.251	0.749	0.516	0.484	104.940	263.774	356.974	47.659	7.471
19	0.203	0.797	0.490	0.510	104.984	263.743	357.792	47.545	7.351
20	0.085	0.915	0.381	0.619	104.953	158.800	361.403	47.255	7.092

Table5.111 Simulation results using N =20 and %AAD of K-value = -9.99%.

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	1.000	0.000	0.5	0.5	100.000	0	300.000	0.000	0.000
2	0.999	0.000	0.5	0.5	100.000	62.49	300.000	0.000	0.000
3	0.999	0.001	0.5	0.5	100.000	62.49	300.000	0.000	0.000
4	0.997	0.003	0.5	0.5	100.000	62.49	300.000	0.000	0.000
5	0.995	0.005	0.5	0.5	100.000	62.49	300.000	0.000	0.000
6	0.990	0.010	0.5	0.5	100.000	62.49	300.000	0.000	0.000
7	0.982	0.018	0.5	0.5	100.000	62.49	300.000	0.000	0.000
8	0.965	0.035	0.5	0.5	100.000	62.49	300.000	0.000	0.000
9	0.936	0.064	0.5	0.5	100.000	62.49	300.000	0.000	0.000
10	0.884	0.116	0.5	0.5	100.000	62.49	300.000	0.000	0.000
11	0.800	0.200	0.5	0.5	100.000	62.49	300.000	0.000	0.000
12	0.678	0.322	0.5	0.5	100.000	62.49	300.000	0.000	0.000
13	0.524	0.476	0.5	0.5	100.000	62.49	300.000	0.000	0.000
14	0.366	0.634	0.5	0.5	100.000	62.49	300.000	0.000	0.000
15	0.232	0.768	0.5	0.5	100.000	258.79	300.000	0.000	0.000
16	0.232	0.768	0.5	0.5	100.000	258.79	300.000	0.000	0.000
17	0.232	0.768	0.5	0.5	100.000	258.79	300.000	0.000	0.000
18	0.233	0.767	0.5	0.5	100.000	258.79	300.000	0.000	0.000
19	0.234	0.766	0.5	0.5	100.000	258.79	300.000	0.000	0.000
20	0.229	0.771	0.5	0.5	100.000	158.80	300.000	0.000	0.000

Table5.111 (continued)

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.797	0.203	0.797	0.203	0.000	64.742	351.200	48.824	8.719
2	0.787	0.213	0.785	0.215	102.252	64.814	351.213	48.761	8.671
3	0.775	0.225	0.774	0.226	102.324	64.876	351.231	48.703	8.625
4	0.762	0.238	0.764	0.236	102.386	64.931	351.253	48.650	8.582
5	0.748	0.252	0.755	0.245	102.441	64.980	351.281	48.602	8.543
6	0.733	0.267	0.747	0.253	102.490	65.029	351.314	48.557	8.505
7	0.718	0.282	0.739	0.261	102.539	65.078	351.355	48.514	8.468
8	0.701	0.299	0.731	0.269	102.588	65.134	351.404	48.471	8.430
9	0.683	0.317	0.723	0.277	102.644	65.201	351.464	48.426	8.389
10	0.661	0.339	0.713	0.287	102.711	65.287	351.543	48.374	8.341
11	0.635	0.365	0.702	0.298	102.797	65.410	351.651	48.309	8.280
12	0.600	0.400	0.686	0.314	102.920	65.600	351.815	48.223	8.195
13	0.547	0.453	0.665	0.335	103.110	65.933	352.097	48.095	8.062
14	0.456	0.544	0.630	0.370	103.443	66.561	352.673	47.882	7.826
15	0.288	0.712	0.571	0.429	104.071	262.666	354.129	47.491	7.363
16	0.288	0.712	0.569	0.431	103.876	262.608	354.141	47.479	7.349
17	0.282	0.718	0.567	0.433	103.818	262.546	354.198	47.465	7.332
18	0.270	0.730	0.564	0.436	103.756	262.600	354.345	47.445	7.308
19	0.226	0.774	0.549	0.451	103.810	262.659	354.926	47.365	7.211
20	0.091	0.909	0.453	0.547	103.869	158.800	358.612	47.096	6.901

Table5.112 Simulation results using N =20 and %AAD of K-value = +22.77%.

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.999	0.000	0.5	0.5	100.000	0	300.000	0.000	0.000
2	0.999	0.000	0.5	0.5	100.000	62.49	300.000	0.000	0.000
3	0.998	0.002	0.5	0.5	100.000	62.49	300.000	0.000	0.000
4	0.997	0.003	0.5	0.5	100.000	62.49	300.000	0.000	0.000
5	0.994	0.006	0.5	0.5	100.000	62.49	300.000	0.000	0.000
6	0.989	0.011	0.5	0.5	100.000	62.49	300.000	0.000	0.000
7	0.979	0.021	0.5	0.5	100.000	62.49	300.000	0.000	0.000
8	0.961	0.039	0.5	0.5	100.000	62.49	300.000	0.000	0.000
9	0.930	0.070	0.5	0.5	100.000	62.49	300.000	0.000	0.000
10	0.876	0.124	0.5	0.5	100.000	62.49	300.000	0.000	0.000
11	0.790	0.210	0.5	0.5	100.000	62.49	300.000	0.000	0.000
12	0.667	0.333	0.5	0.5	100.000	62.49	300.000	0.000	0.000
13	0.516	0.484	0.5	0.5	100.000	62.49	300.000	0.000	0.000
14	0.362	0.638	0.5	0.5	100.000	62.49	300.000	0.000	0.000
15	0.232	0.768	0.5	0.5	100.000	258.79	300.000	0.000	0.000
16	0.232	0.768	0.5	0.5	100.000	258.79	300.000	0.000	0.000
17	0.232	0.768	0.5	0.5	100.000	258.79	300.000	0.000	0.000
18	0.232	0.768	0.5	0.5	100.000	258.79	300.000	0.000	0.000
19	0.234	0.766	0.5	0.5	100.000	258.79	300.000	0.000	0.000
20	0.229	0.771	0.5	0.5	100.000	158.80	300.000	0.000	0.000

Table5.112 (continued)

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.839	0.161	0.879	0.121	0.000	64.742	352.811	49.463	9.068
2	0.789	0.211	0.843	0.157	102.252	64.872	353.173	49.332	8.966
3	0.743	0.257	0.811	0.189	102.382	64.992	353.518	49.216	8.874
4	0.701	0.299	0.783	0.217	102.502	65.107	353.855	49.110	8.787
5	0.661	0.339	0.756	0.244	102.617	65.221	354.190	49.010	8.704
6	0.623	0.377	0.730	0.270	102.731	65.338	354.530	48.912	8.620
7	0.585	0.415	0.705	0.295	102.848	65.458	354.885	48.814	8.534
8	0.546	0.454	0.679	0.321	102.968	65.584	355.263	48.712	8.444
9	0.506	0.494	0.652	0.348	103.094	65.714	355.676	48.606	8.348
10	0.464	0.536	0.625	0.375	103.224	65.846	356.133	48.494	8.244
11	0.421	0.579	0.597	0.403	103.356	65.975	356.643	48.377	8.135
12	0.375	0.625	0.569	0.431	103.485	66.097	357.205	48.257	8.022
13	0.330	0.670	0.542	0.458	103.607	66.214	357.815	48.137	7.907
14	0.287	0.713	0.515	0.485	103.724	66.330	358.463	48.019	7.795
15	0.246	0.754	0.488	0.512	103.840	264.555	359.141	47.903	7.684
16	0.246	0.754	0.488	0.512	105.765	264.590	359.133	47.903	7.684
17	0.244	0.756	0.485	0.515	105.800	264.640	359.173	47.890	7.673
18	0.231	0.769	0.473	0.527	105.850	264.729	359.412	47.841	7.627
19	0.185	0.815	0.436	0.564	105.939	264.703	360.348	47.694	7.493
20	0.085	0.915	0.323	0.677	105.913	158.800	363.558	47.370	7.256

Table5.113 Simulation results using N =20 and %AAD of K-value = -22.20%.

Initiated data:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	1.000	0.000	0.5	0.5	100.000	0	300.000	0.000	0.000
2	0.999	0.000	0.5	0.5	100.000	62.49	300.000	0.000	0.000
3	0.999	0.001	0.5	0.5	100.000	62.49	300.000	0.000	0.000
4	0.998	0.002	0.5	0.5	100.000	62.49	300.000	0.000	0.000
5	0.996	0.004	0.5	0.5	100.000	62.49	300.000	0.000	0.000
6	0.992	0.008	0.5	0.5	100.000	62.49	300.000	0.000	0.000
7	0.984	0.016	0.5	0.5	100.000	62.49	300.000	0.000	0.000
8	0.969	0.031	0.5	0.5	100.000	62.49	300.000	0.000	0.000
9	0.942	0.058	0.5	0.5	100.000	62.49	300.000	0.000	0.000
10	0.893	0.107	0.5	0.5	100.000	62.49	300.000	0.000	0.000
11	0.812	0.188	0.5	0.5	100.000	62.49	300.000	0.000	0.000
12	0.690	0.310	0.5	0.5	100.000	62.49	300.000	0.000	0.000
13	0.534	0.466	0.5	0.5	100.000	62.49	300.000	0.000	0.000
14	0.371	0.629	0.5	0.5	100.000	62.49	300.000	0.000	0.000
15	0.233	0.767	0.5	0.5	100.000	258.79	300.000	0.000	0.000
16	0.233	0.767	0.5	0.5	100.000	258.79	300.000	0.000	0.000
17	0.233	0.767	0.5	0.5	100.000	258.79	300.000	0.000	0.000
18	0.233	0.767	0.5	0.5	100.000	258.79	300.000	0.000	0.000
19	0.235	0.765	0.5	0.5	100.000	258.79	300.000	0.000	0.000
20	0.229	0.771	0.5	0.5	100.000	158.80	300.000	0.000	0.000

Table5.113 (continued)

Finished calculation results:

Stage	x_1	x_2	y_1	y_2	V	L	T	Hv	Hl
1	0.760	0.240	0.750	0.249	0.000	64.742	350.491	48.460	8.481
2	0.740	0.260	0.739	0.261	102.252	64.750	350.508	48.389	8.420
3	0.721	0.279	0.732	0.268	102.260	64.737	350.531	48.347	8.383
4	0.706	0.294	0.729	0.271	102.247	64.718	350.556	48.329	8.367
5	0.695	0.305	0.729	0.271	102.228	64.701	350.575	48.326	8.364
6	0.688	0.312	0.730	0.270	102.211	64.691	350.588	48.331	8.369
7	0.685	0.315	0.731	0.269	102.201	64.694	350.594	48.337	8.374
8	0.683	0.317	0.731	0.269	102.204	64.713	350.598	48.340	8.377
9	0.681	0.319	0.730	0.270	102.223	64.755	350.603	48.334	8.371
10	0.676	0.324	0.727	0.273	102.265	64.827	350.617	48.314	8.354
11	0.665	0.335	0.720	0.280	102.337	64.949	350.647	48.275	8.317
12	0.644	0.356	0.709	0.291	102.459	65.156	350.713	48.204	8.249
13	0.602	0.398	0.689	0.311	102.666	65.546	350.864	48.081	8.125
14	0.512	0.488	0.656	0.344	103.056	66.395	351.273	47.851	7.871
15	0.301	0.699	0.594	0.406	103.905	261.851	352.712	47.364	7.275
16	0.298	0.702	0.592	0.408	103.061	261.774	352.740	47.352	7.260
17	0.291	0.709	0.591	0.409	102.984	261.713	352.800	47.343	7.248
18	0.281	0.719	0.590	0.410	102.923	261.820	352.899	47.338	7.242
19	0.246	0.754	0.582	0.418	103.030	262.073	353.290	47.280	7.169
20	0.102	0.898	0.498	0.502	103.283	158.800	356.666	46.996	6.802

Table5.114 %AAD of composition (x_1) profile by varying number of stage at %AAD of K-value =+ 9.25%.

Stage	$X_{1N=20}$	$X_{1N=20(+9.25\%)}$	Δ	$X_{1N=14}$	$X_{1N=14(+9.25\%)}$	Δ	$X_{1N=10}$	$X_{1N=10(+9.25\%)}$	Δ
1	0.800	0.826	0.0325	0.786	0.807	0.0267	0.773	0.773	0.0000
2	0.779	0.798	0.0244	0.755	0.773	0.0238	0.731	0.719	0.0164
3	0.761	0.772	0.0145	0.725	0.741	0.0221	0.685	0.665	0.0292
4	0.743	0.748	0.0067	0.696	0.709	0.0187	0.635	0.609	0.0409
5	0.727	0.724	0.0041	0.667	0.676	0.0135	0.576	0.548	0.0486
6	0.709	0.700	0.0127	0.637	0.639	0.0031	0.506	0.477	0.0573
7	0.691	0.675	0.0232	0.602	0.595	0.0116	0.411	0.387	0.0584
8	0.67	0.648	0.0328	0.56	0.539	0.0375	0.267	0.263	0.0150
9	0.647	0.619	0.0433	0.502	0.468	0.0677	0.231	0.225	0.0260
10	0.619	0.586	0.0533	0.413	0.377	0.0872	0.104	0.103	0.0096
11	0.585	0.549	0.0615	0.274	0.266	0.0292			
12	0.542	0.503	0.0720	0.268	0.254	0.0522			
13	0.484	0.445	0.0806	0.231	0.208	0.0996			
14	0.399	0.368	0.0777	0.101	0.089	0.1188			
15	0.27	0.267	0.0111						
16	0.27	0.268	0.0074						
17	0.272	0.265	0.0257						
18	0.27	0.251	0.0704						
19	0.232	0.203	0.1250						
20	0.099	0.085	0.1414						
Sum of data			0.9203			0.6118			0.3014

N = number of data points

$$\Delta = \left| \frac{x_{1at\ \%AAD} - x_{1accurate}}{x_{1accurate}} \right|$$

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N} \left| \frac{x_{1at\ \%AAD} - x_{1accurate}}{x_{1accurate}} \right| \right] x100$$

At n=20 and +9.25%AAD of K-value = (0.9203x100)/20

= 4.60%

At n=14 and +9.25%AAD of K-value = (0.6188x100)/14

= 4.42%

At n=10 and +9.25%AAD of K-value = (0.3014x100)/10

= 3.01%

Table5.115 %AAD of liquid composition (x_1) profile by varying number of stage at %AAD of K-value=+22.77%.

Stage	$X_{1N=20}$	$X_{1N=20(+22.77\%)}$	Δ	$X_{1N=14}$	$X_{1N=14(+22.77\%)}$	Δ	$X_{1N=10}$	$X_{1N=10(+22.77\%)}$	Δ
1	0.800	0.839	0.0487	0.786	0.812	0.0331	0.773	0.776	0.0039
2	0.779	0.789	0.0128	0.755	0.748	0.0093	0.731	0.696	0.0479
3	0.761	0.743	0.0237	0.725	0.688	0.0510	0.685	0.620	0.0949
4	0.743	0.701	0.0565	0.696	0.63	0.0948	0.635	0.545	0.1417
5	0.727	0.661	0.0908	0.667	0.574	0.1394	0.576	0.472	0.1806
6	0.709	0.623	0.1213	0.637	0.517	0.1884	0.506	0.398	0.2134
7	0.691	0.585	0.1534	0.602	0.462	0.2326	0.411	0.322	0.2165
8	0.670	0.546	0.1851	0.560	0.407	0.2732	0.267	0.244	0.0861
9	0.647	0.506	0.2179	0.502	0.353	0.2968	0.231	0.202	0.1255
10	0.619	0.464	0.2504	0.413	0.300	0.2736	0.104	0.101	0.0288
11	0.585	0.421	0.2803	0.274	0.245	0.1058			
12	0.542	0.375	0.3081	0.268	0.233	0.1306			
13	0.484	0.330	0.3182	0.231	0.193	0.1645			
14	0.399	0.287	0.2807	0.101	0.094	0.0693			
15	0.270	0.246	0.0889						
16	0.270	0.246	0.0889						
17	0.272	0.244	0.1029						
18	0.270	0.231	0.1444						
19	0.232	0.185	0.2026						
20	0.099	0.085	0.1414						
Sum of data			3.1172			2.0625			1.1395

N = number of data points

$$\Delta = \left| \frac{x_{1\text{at }\%AAD} - x_{1accurate}}{x_{1accurate}} \right|$$

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\frac{x_{1\text{at }\%AAD} - x_{1accurate}}{x_{1accurate}}\right|\right]x100$$

At n=20 and +22.77%AAD of K-value = (3.1172x100)/20

= 15.59%

At n=14 and +22.77%AAD of K-value = (2.0625x100)/14

= 14.7%

At n=10 and +22.77%AAD of K-value = (1.1395x100)/10

= 11.35%

Table5.116 %AAD of liquid composition (x_1) profile by varying number of stage at %AAD of K-value=-9.99%.

Stage	$X_{1N=20}$	$X_{1N=20(-9.99\%)}$	Δ	$X_{1N=14}$	$X_{1N=14(-9.99\%)}$	Δ	$X_{1N=10}$	$X_{1N=10(-9.99\%)}$	Δ
1	0.800	0.797	0.0038	0.786	0.785	0.0013	0.773	0.770	0.0039
2	0.779	0.787	0.0103	0.755	0.777	0.0291	0.731	0.752	0.0287
3	0.761	0.775	0.0184	0.725	0.765	0.0552	0.685	0.729	0.0642
4	0.743	0.762	0.0256	0.696	0.749	0.0761	0.635	0.696	0.0961
5	0.727	0.748	0.0289	0.667	0.729	0.0930	0.576	0.648	0.1250
6	0.709	0.733	0.0339	0.637	0.702	0.1020	0.506	0.576	0.1383
7	0.691	0.718	0.0391	0.602	0.668	0.1096	0.411	0.464	0.1290
8	0.670	0.701	0.0463	0.560	0.622	0.1107	0.267	0.279	0.0449
9	0.647	0.683	0.0556	0.502	0.559	0.1135	0.231	0.237	0.0260
10	0.619	0.661	0.0679	0.413	0.459	0.1114	0.104	0.097	0.0673
11	0.585	0.635	0.0855	0.274	0.286	0.0438			
12	0.542	0.600	0.1070	0.268	0.277	0.0336			
13	0.484	0.547	0.1302	0.231	0.233	0.0087			
14	0.399	0.456	0.1429	0.101	0.093	0.0792			
15	0.270	0.288	0.0667						
16	0.270	0.288	0.0667						
17	0.272	0.282	0.0368						
18	0.270	0.270	0.0000						
19	0.232	0.226	0.0259						
20	0.099	0.091	0.0808						
Sum of data			1.0718			0.9672			0.7234

N = number of data points

$$\Delta = \left| \frac{x_{1at\ \%AAD} - x_{1accurate}}{x_{1accurate}} \right|$$

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\frac{x_{1at\ \%AAD} - x_{1accurate}}{x_{1accurate}}\right|\right]x100$$

At n=20 and –9.99%AAD of K-value = (1.0718x100)/20

= 5.36%

At n=14 and –9.99%AAD of K-value = (0.9672x100)/14

= 6.91%

At n=10 and –9.99%AAD of K-value = (0.7234x100)/10

= 7.23%

Table5.117 %AAD of liquid composition (x_1) profile by varying number of stage at %AAD of K-value=-22.20%.

Stage	$X_{1N=20}$	$X_{1N=20(-22.20\%)}$	Δ	$X_{1N=14}$	$X_{1N=14(-22.20\%)}$	Δ	$X_{1N=10}$	$X_{1N=10(-22.20\%)}$	Δ
1	0.800	0.760	0.0500	0.786	0.724	0.0789	0.773	0.724	0.0634
2	0.779	0.740	0.0501	0.755	0.715	0.0530	0.731	0.699	0.0438
3	0.761	0.721	0.0526	0.725	0.712	0.0179	0.685	0.680	0.0073
4	0.743	0.706	0.0498	0.696	0.712	0.0230	0.635	0.662	0.0425
5	0.727	0.695	0.0440	0.667	0.711	0.0660	0.576	0.640	0.1111
6	0.709	0.688	0.0296	0.637	0.706	0.1083	0.506	0.601	0.1877
7	0.691	0.685	0.0087	0.602	0.692	0.1495	0.411	0.514	0.2506
8	0.670	0.683	0.0194	0.560	0.666	0.1893	0.267	0.300	0.1236
9	0.647	0.681	0.0526	0.502	0.617	0.2291	0.231	0.271	0.1732
10	0.619	0.676	0.0921	0.413	0.519	0.2567	0.104	0.115	0.1058
11	0.585	0.665	0.1368	0.274	0.303	0.1058			
12	0.542	0.644	0.1882	0.268	0.304	0.1343			
13	0.484	0.602	0.2438	0.231	0.274	0.1861			
14	0.399	0.512	0.2832	0.101	0.113	0.1188			
15	0.270	0.301	0.1148						
16	0.270	0.298	0.1037						
17	0.272	0.291	0.0699						
18	0.270	0.281	0.0407						
19	0.232	0.246	0.0603						
20	0.099	0.102	0.0303						
Sum of data			1.7205			1.7167			1.1090

N = number of data points

$$\Delta = \left| \frac{x_{1\text{at }\%\text{AAD}} - x_{1\text{accurate}}}{x_{1\text{accurate}}} \right|$$

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\frac{x_{1\text{at }\%\text{AAD}} - x_{1\text{accurate}}}{x_{1\text{accurate}}}\right|\right] \text{x100}$$

At n=20 and –22.20%AAD of K-value = (1.7205x100)/20

= 8.60%

At n=14 and –22.20%AAD of K-value = (1.7167x100)/14

= 12.26%

At n=10 and –22.20%AAD of K-value = (1.1090x100)/10

= 11.09%

Table5.118 %AAD of temperature profile by varying number of stage at %AAD of K-value=+9.25%.

Stage	$T_{N=20}$	$T_{N=20(+9.25\%)}$	Δ	$T_{N=14}$	$T_{N=14(+9.25\%)}$	Δ	$T_{N=10}$	$T_{N=10(+9.25\%)}$	Δ
1	351.786	352.184	0.0011	351.827	352.255	0.0012	351.867	352.409	0.0015
2	351.840	352.297	0.0013	351.921	352.403	0.0014	352.012	352.674	0.0019
3	351.896	352.410	0.0015	352.028	352.557	0.0015	352.203	352.982	0.0022
4	351.955	352.526	0.0016	352.147	352.724	0.0016	352.457	353.348	0.0025
5	352.018	352.649	0.0018	352.282	352.915	0.0018	352.799	353.800	0.0028
6	352.088	352.782	0.0020	352.439	353.149	0.0020	353.280	354.390	0.0031
7	352.169	352.928	0.0022	352.634	353.454	0.0023	354.048	355.265	0.0034
8	352.266	353.094	0.0024	352.898	353.873	0.0028	355.597	356.787	0.0033
9	352.386	353.286	0.0026	353.304	354.476	0.0033	356.113	357.392	0.0036
10	352.538	353.514	0.0028	354.027	355.372	0.0038	359.318	360.556	0.0034
11	352.739	353.796	0.0030	355.505	356.752	0.0035			
12	353.019	354.166	0.0032	355.582	356.923	0.0038			
13	353.442	354.684	0.0035	356.110	357.704	0.0045			
14	354.158	355.472	0.0037	359.443	361.239	0.0050			
15	355.559	356.730	0.0033						
16	355.556	356.721	0.0033						
17	355.527	356.769	0.0035						
18	355.557	356.974	0.0040						
19	356.099	357.792	0.0048						
20	359.551	361.403	0.0052						
Sum of data			0.0565			0.0385			0.0280

N = number of data points

$$\Delta = \left| \frac{T_{\text{at \%AAD}} - T_{\text{accurate}}}{T_{\text{accurate}}} \right|$$

$$\text{\%Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N}\left|\frac{T_{\text{at \%AAD}} - T_{\text{accurate}}}{T_{\text{accurate}}}\right|\right]\text{x}100$$

At n=20 and +9.25%AAD of K-value = (0.0565x100)/20

= 0.28%

At n=14 and +9.25%AAD of K-value = (0.0385x100)/14

= 0.28%

At n=10 and +9.25%AAD of K-value = (0.0280x100)/10

= 0.28%

Table5.119 %AAD of temperature profile by varying number of stage at %AAD of K-value = +22.77%.

Stage	$T_{N=20}$	$T_{N=20(+22.77\%)}$	Δ	$T_{N=14}$	$T_{N=14(+22.77\%)}$	Δ	$T_{N=10}$	$T_{N=10(+22.77\%)}$	Δ
1	351.786	352.811	0.0029	351.827	353.009	0.0034	351.867	353.268	0.0040
2	351.840	353.173	0.0038	351.921	353.487	0.0044	352.012	353.896	0.0054
3	351.896	353.518	0.0046	352.028	353.968	0.0055	352.203	354.558	0.0067
4	351.955	353.855	0.0054	352.147	354.467	0.0066	352.457	355.272	0.0080
5	352.018	354.190	0.0062	352.282	354.995	0.0077	352.799	356.050	0.0092
6	352.088	354.530	0.0069	352.439	355.559	0.0089	353.280	356.916	0.0103
7	352.169	354.885	0.0077	352.634	356.162	0.0100	354.048	357.926	0.0110
8	352.266	355.263	0.0085	352.898	356.805	0.0111	355.597	359.179	0.0101
9	352.386	355.676	0.0093	353.304	357.493	0.0119	356.113	359.973	0.0108
10	352.538	356.133	0.0102	354.027	358.256	0.0119	359.318	362.840	0.0098
11	352.739	356.643	0.0111	355.505	359.161	0.0103			
12	353.019	357.205	0.0119	355.582	359.371	0.0107			
13	353.442	357.815	0.0124	356.110	360.171	0.0114			
14	354.158	358.463	0.0122	359.443	363.108	0.0102			
15	355.559	359.141	0.0101						
16	355.556	359.133	0.0101						
17	355.527	359.173	0.0103						
18	355.557	359.412	0.0108						
19	356.099	360.348	0.0119						
20	359.551	363.558	0.0111						
Sum of data			0.1773			0.1239			0.0852

N = number of data points

$$\Delta = \left| \frac{T_{\text{at }\%AAD} - T_{\text{accurate}}}{T_{\text{accurate}}} \right|$$

$$\%\text{Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N} \left| \frac{T_{\text{at }\%AAD} - T_{\text{accurate}}}{T_{\text{accurate}}} \right| \right] \text{x}100$$

At n=20 and +22.77%AAD of K-value = (0.1773x100)/20

= 0.89%

At n=14 and +22.77%AAD of K-value = (0.1239x100)/14

= 0.89%

At n=10 and +22.77%AAD of K-value = (0.0852x100)/10

= 0.85%

Table5.120 %AAD of temperature profile by varying number of stage at %AAD of K-value = -9.99%.

Stage	$T_{N=20}$	$T_{N=20(-9.99\%)}$	Δ	$T_{N=14}$	$T_{N=14(-9.99\%)}$	Δ	$T_{N=10}$	$T_{N=10(-9.99\%)}$	Δ
1	351.786	351.200	0.0017	351.827	351.205	0.0018	351.867	351.227	0.0018
2	351.840	351.213	0.0018	351.921	351.220	0.0020	352.012	351.262	0.0021
3	351.896	351.231	0.0019	352.028	351.242	0.0022	352.203	351.320	0.0025
4	351.955	351.253	0.0020	352.147	351.275	0.0025	352.457	351.419	0.0029
5	352.018	351.281	0.0021	352.282	351.325	0.0027	352.799	351.599	0.0034
6	352.088	351.314	0.0022	352.439	351.402	0.0029	353.280	351.938	0.0038
7	352.169	351.355	0.0023	352.634	351.521	0.0032	354.048	352.619	0.0040
8	352.266	351.404	0.0024	352.898	351.711	0.0034	355.597	354.232	0.0038
9	352.386	351.464	0.0026	353.304	352.032	0.0036	356.113	354.771	0.0038
10	352.538	351.543	0.0028	354.027	352.652	0.0039	359.318	358.296	0.0028
11	352.739	351.651	0.0031	355.505	354.152	0.0038			
12	353.019	351.815	0.0034	355.582	354.256	0.0037			
13	353.442	352.097	0.0038	356.110	354.824	0.0036			
14	354.158	352.673	0.0042	359.443	358.488	0.0027			
15	355.559	354.129	0.0040						
16	355.556	354.141	0.0040						
17	355.527	354.198	0.0037						
18	355.557	354.345	0.0034						
19	356.099	354.926	0.0033						
20	359.551	358.612	0.0026						
Sum of data			0.0574			0.0419			0.0311

N = number of data points

$$\Delta = \left| \frac{T_{\text{at \%AAD}} - T_{\text{accurate}}}{T_{\text{accurate}}} \right|$$

%Average Absolute Deviation = $\frac{1}{N}\left[\sum_{N} \left| \frac{T_{\text{at \%AAD}} - T_{\text{accurate}}}{T_{\text{accurate}}} \right| \right]$x100

At n=20 and –9.99%AAD of K-value = (0.0574x100)/20

= 0.29%

At n=14 and –9.99%AAD of K-value = (0.0419x100)/14

= 0.30%

At n=10 and –9.99%AAD of K-value = (0.0311x100)/10

= 0.31%

Table5.121 %AAD of temperature profile by varying number of stage at %AAD of K-value=-22.20%.

Stage	$T_{N=20}$	$T_{N=20(-22.20\%)}$	Δ	$T_{N=14}$	$T_{N=14(-22.20\%)}$	Δ	$T_{N=10}$	$T_{N=10(-22.20\%)}$	Δ
1	351.786	350.491	0.0037	351.827	350.517	0.0037	351.867	350.523	0.0038
2	351.840	350.508	0.0038	351.921	350.526	0.0040	352.012	350.563	0.0041
3	351.896	350.531	0.0039	352.028	350.527	0.0043	352.203	350.604	0.0045
4	351.955	350.556	0.0040	352.147	350.526	0.0046	352.457	350.650	0.0051
5	352.018	350.575	0.0041	352.282	350.528	0.0050	352.799	350.718	0.0059
6	352.088	350.588	0.0043	352.439	350.541	0.0054	353.280	350.862	0.0068
7	352.169	350.594	0.0045	352.634	350.572	0.0058	354.048	351.258	0.0079
8	352.266	350.598	0.0047	352.898	350.643	0.0064	355.597	352.715	0.0081
9	352.386	350.603	0.0051	353.304	350.807	0.0071	356.113	353.001	0.0087
10	352.538	350.617	0.0054	354.027	351.239	0.0079	359.318	356.112	0.0089
11	352.739	350.647	0.0059	355.505	352.691	0.0079			
12	353.019	350.713	0.0065	355.582	352.681	0.0082			
13	353.442	350.864	0.0073	356.110	352.978	0.0088			
14	354.158	351.273	0.0081	359.443	356.173	0.0091			
15	355.559	352.712	0.0080						
16	355.556	352.740	0.0079						
17	355.527	352.800	0.0077						
18	355.557	352.899	0.0075						
19	356.099	353.290	0.0079						
20	359.551	356.666	0.0080						
Sum of data			0.1183			0.0881			0.0640

N = number of data points

$$\Delta = \left| \frac{T_{\text{at \%AAD}} - T_{\text{accurate}}}{T_{\text{accurate}}} \right|$$

$$\text{\%Average Absolute Deviation} = \frac{1}{N}\left[\sum_{N} \left| \frac{T_{\text{at \%AAD}} - T_{\text{accurate}}}{T_{\text{accurate}}} \right| \right] \text{x}100$$

At n=20 and –22.20%AAD of K-value = (0.1183x100)/20

= 0.59%

At n=14 and –22.20%AAD of K-value = (0.0811x100)/14

= 0.58%

At n=10 and –22.20%AAD of K-value = (0.0640x100)/10

= 0.64%

VITA

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