CHAPTER IV

THE PROPOSED GENERAL MODEL

4.1 Rationale

a) Most of components in all natural gases are from the alkanes (or paraffin) series, with the formula C_nH_{2n+2}. The simplest member of the alkane series, methane (CH_4) is generally by far the most abundant component and is always present mostly in gaseous form, ethane (C_2H_6),propane (C_3H_8), and the butanes (C_4H_{10}) may occur in gaseous of liquid forms, depending on the pressure and temperature conditions; while the pentanes (C_5H_{12}), hexanes (C_6H_{14}), heptanes (C_7H_{16}) and heavier components, if present, are always liquids. In general, the higher the boiling point, the smaller will be the proportion of a paraffin in a natural gas mixtures. Several non-hydrocarbon gases also occur in natural gas. All are incombustible, and some may be found in substantial proportions (i.e. nitrogen, hydrogen sulfide, and carbon dioxide). These components have similarity in physical and chemical properties, especially heavy components.

b) Vapor liquid equilibrium K values are used for calculation where liquid and vapor phases coexists. The performance of gas liquid surface separation equipment and separation process in natural gas plants and refineries are predicted using K values. K values are functions of temperature, pressure, liquid phase composition (x_1), and vapor phase composition (y_1). At low and

moderate pressures, the composition effect on K values are small and often can be neclected. Therefore, K values are function of temperature and pressure. (10)

$$K = f(T,P) \qquad (4.1)$$

c) For non-hydrocarbon components (up to 15 mole% nitrogen, 15 mole% carbon dioxide and 15 mole% hydrogen sulfide), they do not affect the K values of the hydrocarbon components except at high pressures.

d) K values can be satisfactorily estimated by multicomponent calculation with the aid of equations of state with their mixing rules.

From the above statements, it is proposed here that some of the components in natural gas can be grouped and be represented by a single component which is to be called "pseudocomponent". For example, a heavy pseucomponent may include components from C_M to C_N, M and N is the first and last components to be included.

4.2 Basis

The model to be developed will be based on the following equations :

a) For vapor liquid equilibrium in a multicomponent system

$$\bar{f}_i^L = \bar{f}_i^V \qquad (4.2)$$

From Equations (2.7) and (2.9)

$$K_i = y_1/x_1 = \bar{\Phi}_i^L / \bar{\Phi}_1^V \qquad (4.3)$$

b) For flash calculations, liquid and vapor phase compositions can be calculated from

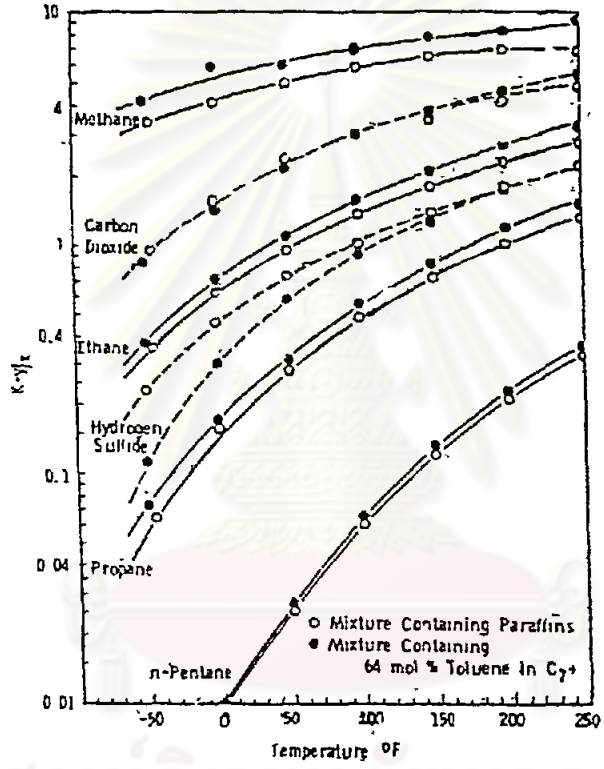

FIGURE 4.1 EFFECT OF TEMPERATURE AND MOLECULAR TYPE ON VAPOR-LIQUID EQUILIBRIUM K VALUES AT 500 PSIA (39)

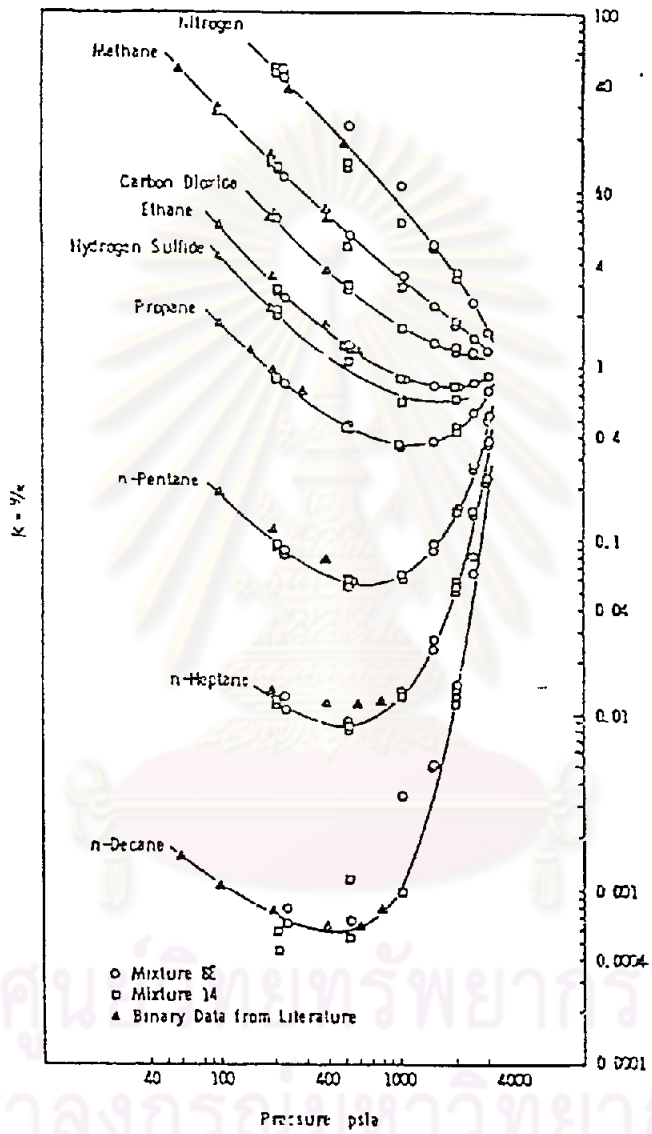

FIGURE 4.2 EFFECT OF PRESSURE ON VAPOR-LIQUID EQUILIBRIUM AT 100°F (39)

$$x_i = \frac{z_i}{(K_i-1)(V/F)+1} \quad (4.4)$$

$$y_i = K_i x_i \quad (4.5)$$

c) The Soave Redlich Kwong equation of state (Equation 4.7) is used for K values calculation. The same equation of state is used for both phases, a fugacity coefficient can be estimated for both vapor (V) and liquid (L) from the SRK equation of state which is

$$\ln \bar{\Phi}_i = (b_i/b)(Z-1)-\ln(Z-B)-(A/B)[\{2(ac\alpha)_i/(ac\alpha)\}-(b_i/b)]\ln(1+B/Z) \quad (4.6)$$

$$Z^3-Z^2+(A-B-B^2)Z-AB = 0 \quad (4.7)$$

where

$$A = (ac\alpha)P/R^2T^2 \quad (4.8)$$

$$B = Pb/RT \quad (4.9)$$

$$b_i = \Omega_b RTC_i/PC_i \quad (4.10)$$

$$b = \sum_{i=1}^{N} x_i b_i \quad (4.11)$$

$$ac_i = \Omega_a R^2 TC_i^2/PC_i \quad (4.12)$$

$$\alpha_i^{1/2} = 1 + m_i(1-TR_i^{1/2}) \quad (4.13)$$

$$(ac\alpha) = \sum_{ij}^{N}\sum x_i x_j ac_i^{1/2} ac_j^{1/2} \alpha_i^{1/2} \alpha_j^{1/2} (1-k_{ij}) \quad (4.14)$$

$$(ac\alpha)_i = \sum_{j=1}^{N} x_i ac_i^{1/2} ac_j^{1/2} \alpha_i^{1/2} \alpha_j^{1/2} (1-k_{ij}) \quad (4.15)$$

$$m_i = 0.480 + 1.574\omega_i + 0.176\omega_i^2 \quad (4.16)$$

$$\Omega_a = 0.42747 \qquad \Omega_b = 0.08664$$

d) For finding (V/F) in the flash calculation, the Newton Raphson method is applied because of rapid convergence. The Newton Raphson method provides the following equation

$$(V/F)_{new} = (V/F) - \frac{F(V/F)}{F'(V/F)} \quad (4.17)$$

4.3 Algorithm

The algorithm of the proposed model is as follows :

1. Select components to be included in the pseudocomponents

a) Light Pseudocomponent (C_{M-})

For example, components included may be C_1, C_2 and C_3 or in general form : $C_1, C_2, \ldots, C_{M-1}$

Component	Eq. to be satisfied			Component	Eq. to be satisfied		
CO_2	y_{CO_2}	=	$K_{CO_2} x_{CO_2}$	CO_2	y_{CO_2}	=	$K_{CO_2} x_{CO_2}$
N_2	y_{N_2}	=	$K_{N_2} x_{N_2}$	N_2	y_{N_2}	=	$K_{N_2} x_{N_2}$
C_1	y_{C_1}	=	$K_{C_1} x_{C_1}$	C_{4-}	$y_{C_{4-}}$	=	$K_{C_{4-}} x_{C_{4-}}$
C_2	y_{C_2}	=	$K_{C_2} x_{C_2}$				
C_3	y_{C_3}	=	$K_{C_3} x_{C_3}$				
i-C_4	y_{iC_4}	=	$K_{iC_4} x_{iC_4}$	i-C_4	y_{iC_4}	=	$K_{iC_4} x_{iC_4}$
.	.			.	.		
.	.			.	.		
.	.			.	.		
C_N	y_{C_N}	=	$K_{C_N} x_{C_N}$	C_N	y_{C_N}	=	$K_{C_N} x_{C_N}$

b) Heavy Pseudocomponent (C_{M+})

For example, components included may be i C_4, n C_4, i $C_5, \ldots, C_N$ or in general form : $C_M, C_{M+1}, C_{M+2}, \ldots, C_N$

Component	Eq. to be satisfied			Component	Eq. to be satisfied		
CO_2	y_{CO_2}	=	$K_{CO_2} x_{CO_2}$	CO_2	y_{CO_2}	=	$K_{CO_2} x_{CO_2}$
N_2	y_{N_2}	=	$K_{N_2} x_{N_2}$	N_2	y_{N_2}	=	$K_{N_2} x_{N_2}$
C_1	y_{C_1}	=	$K_{C_1} x_{C_1}$	C_1	y_{C_1}	=	$K_{C_1} x_{C_1}$
C_2	y_{C_2}	=	$K_{C_2} x_{C_2}$	C_2	y_{C_2}	=	$K_{C_2} x_{C_2}$
C_3	y_{C_3}	=	$K_{C_3} x_{C_3}$	C_3	y_{C_3}	=	$K_{C_3} x_{C_3}$
i-C_4	y_{iC_4}	=	$K_{iC_4} x_{iC_4}$	C_{4+}	$y_{C_{4+}}$	=	$K_{C_{4+}} x_{C_{4+}}$
.	.						
.	.						
C_N	y_{C_N}	=	$K_{C_N} x_{C_N}$				

2. Initial estimate of the phase compositions (x_i, y_i)

a) Let the second heavy component (M+1) in the heavy pseudocomponent represent the heavy pseudocomponent;

$$TC_{1,ps} = TC_{(M+1)} \quad (4.18)$$

$$PC_{1,ps} = PC_{(M+1)} \quad (4.19)$$

$$\omega_{1,ps} = \omega_{(M+1)} \quad (4.20)$$

b) assume $y_1 = z_1$

c) For liquid phase composition (x_i)

$$x_i = 1.0/N \quad (4.21)$$

3. Perform flash calculation to obtain phase compositions of components in the light pseudocomponent, CO_2, N_2

i.e. $x_{CO_2}, x_{N_2}, x_{C_1}, x_{C_2}, \ldots, x_{C_{M-1}}$

$y_{CO_2}, y_{N_2}, y_{C_1}, y_{C_2}, \ldots, y_{C_{M-1}}$

4. Calculate the properties of the light pseudocomponent of known compositions by using the Kay's rule

$$TC_{1,ps} = \Sigma\, x_1 TC_1 \quad (4.22)$$

$$PC_{i,ps} = \Sigma\, x_i PC_1 \quad (4.23)$$

$$\omega_{1,ps} = \Sigma\, x_i \omega_1 \quad (4.24)$$

5. Perform flash calculation to obtain phase compositions of components in the heavy pseudocomponent

i.e. $x_{C_M}, x_{C_{M+1}}, \ldots, x_{C_N}$

$y_{C_M}, y_{C_{M+1}}, \ldots, y_{C_N}$

6. Calculate the properties of the heavy pseudocomponent of known composition by the Kay's rule

$$TC_{i,ps} = \Sigma\, x_i TC_1 \quad (4.25)$$

$$PC_{i,ps} = \Sigma\, x_1 PC_1 \quad (4.26)$$

$$\omega_{i,ps} = \Sigma\, x_1 \omega_i \quad (4.27)$$

7. Repeat step 3, then the liquid and vapor phase compositions of all components in the natural gas are known,

$$x_{CO_2},\ x_{N_2},\ x_{C_1},\ \cdots,\ x_{C_N}$$

and $$y_{CO_2},\ y_{N_2},\ y_{C_1},\ \cdots,\ y_{C_N}$$

The flow diagram of the calculation is presented in Figure 4.4.

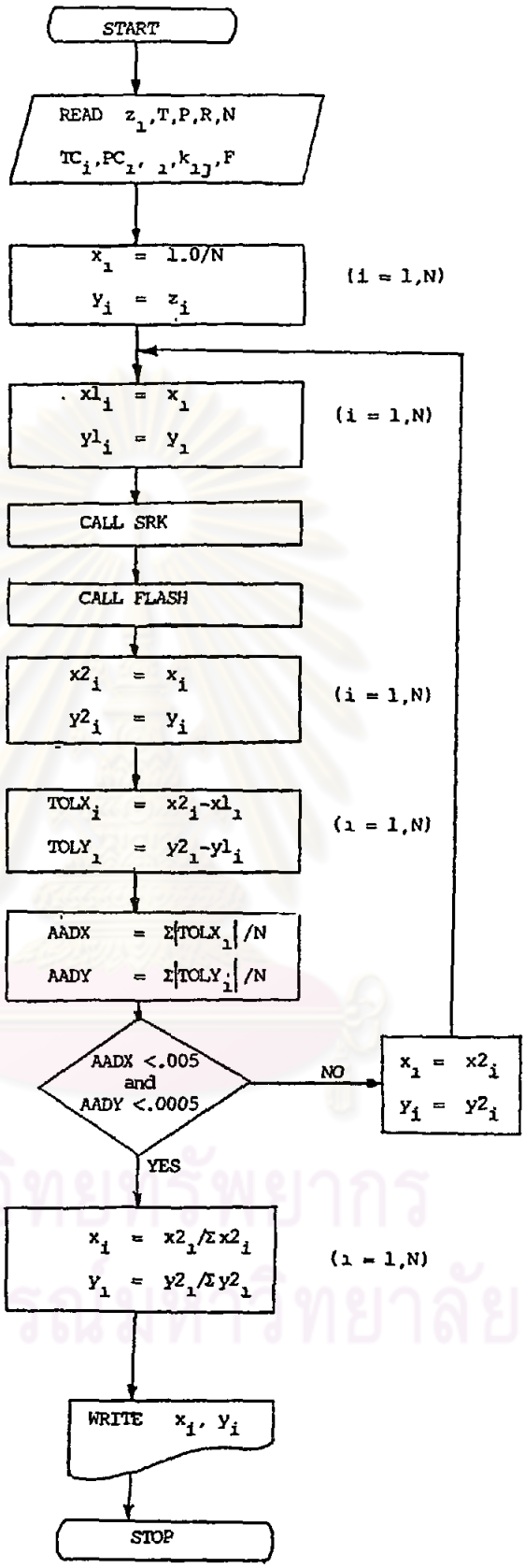

FIGURE 4.3 ALGORITHM OF THE ORDINARY VLE CALCULATION MODEL

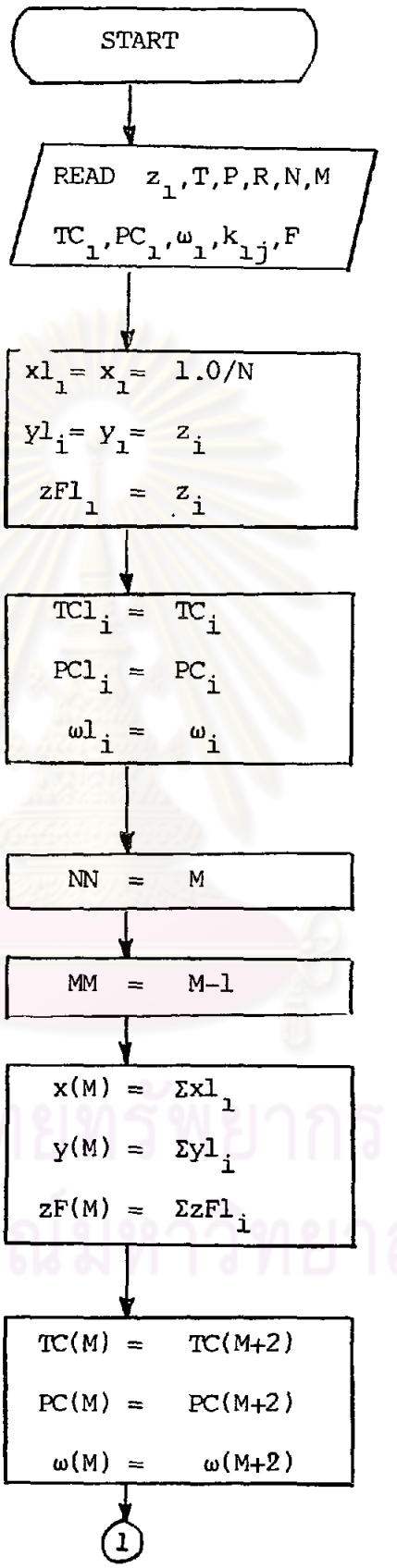

FIGURE 4.4 ALGORITHM OF THE PROPOSED GENERAL MODEL

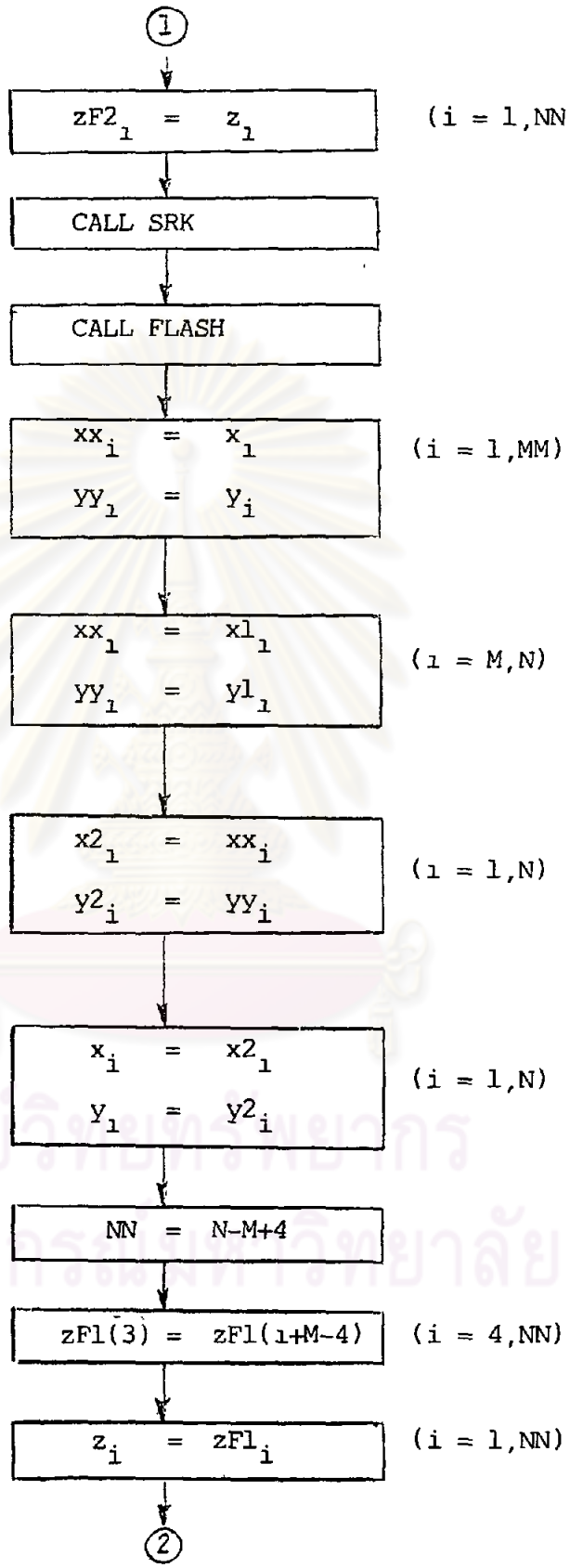

FIGURE 4.4 ALGORITHM OF THE PROPOSED GENERAL MODEL (CONTINUED)

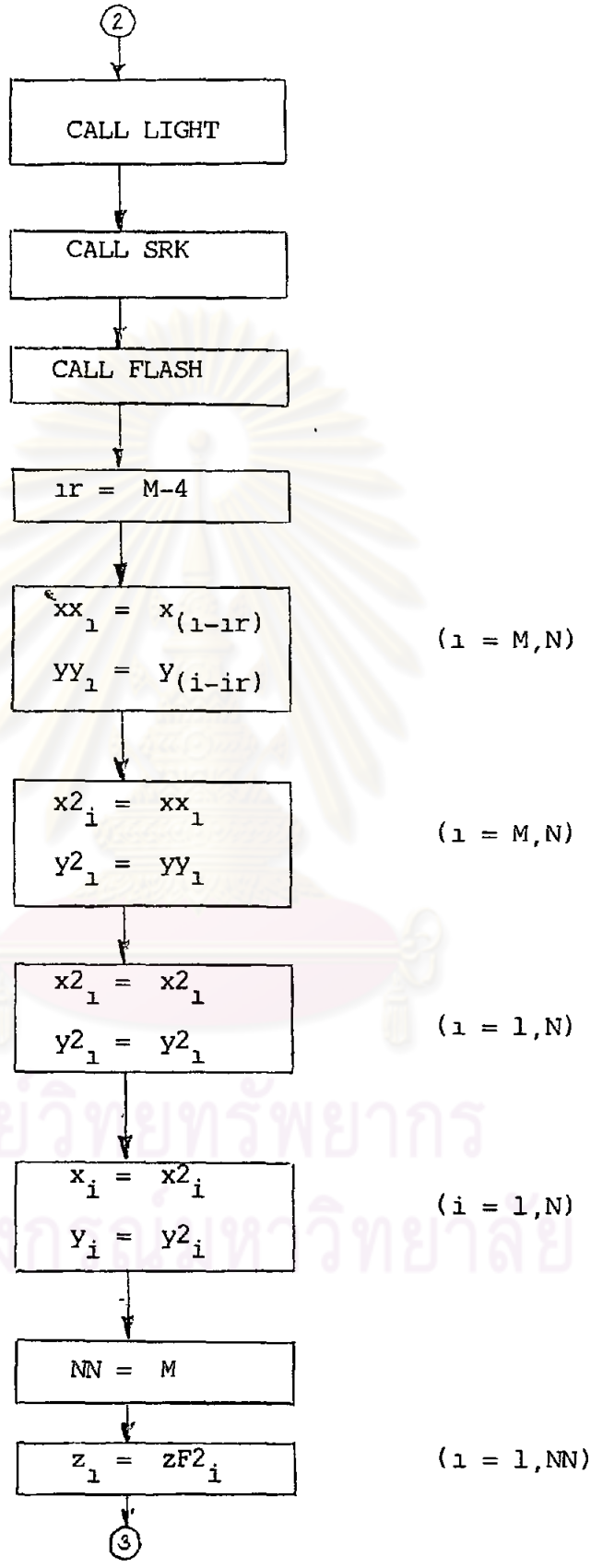

FIGURE 4.4 ALGORITHM OF THE PROPOSED GENERAL MODEL (CONTINUED)

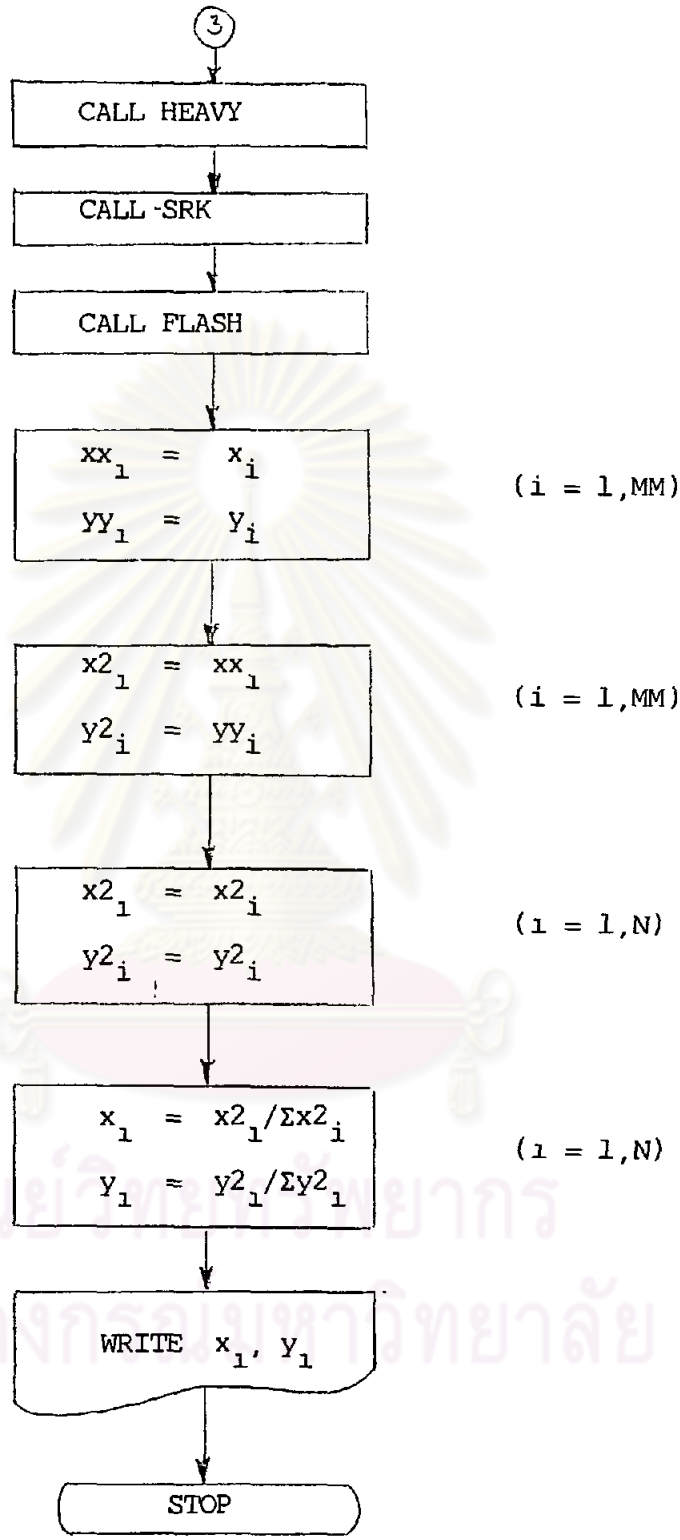

FIGURE 4.4 ALGORITHM OF THE PROPOSED GENERAL MODEL (CONTINUED)

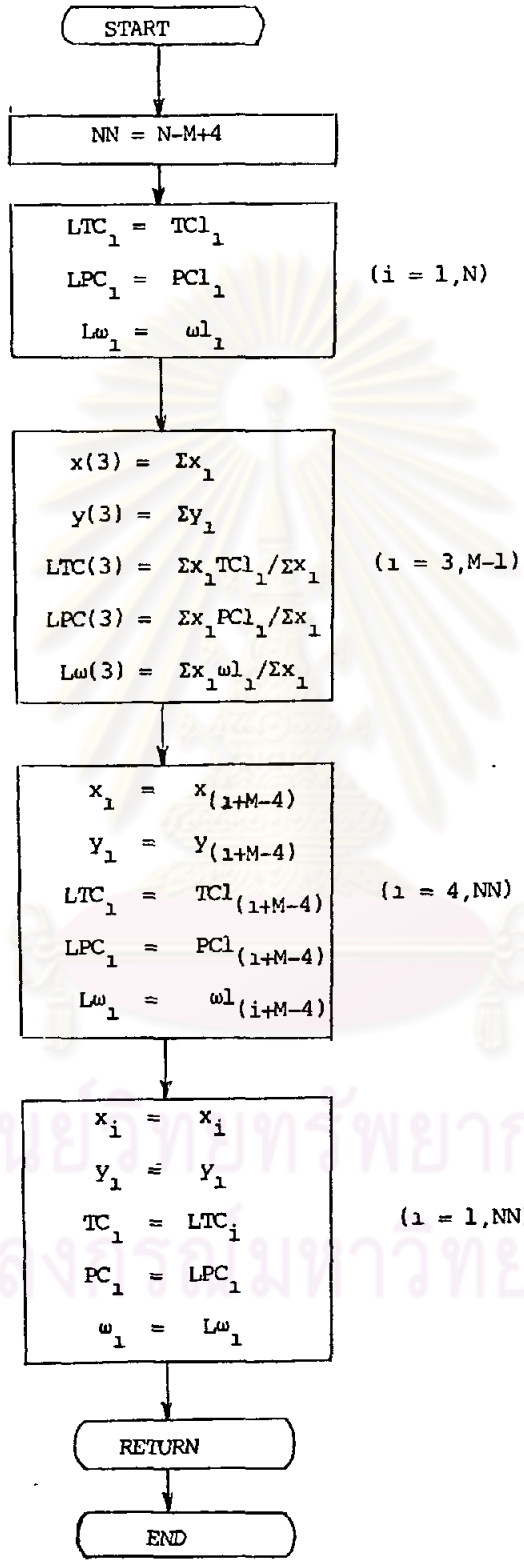

FIGURE 4.5 ALGORITHM FOR GROUPING LIGHT-PSEUDOCOMPONENT (SUBROUTINE LIGHT)

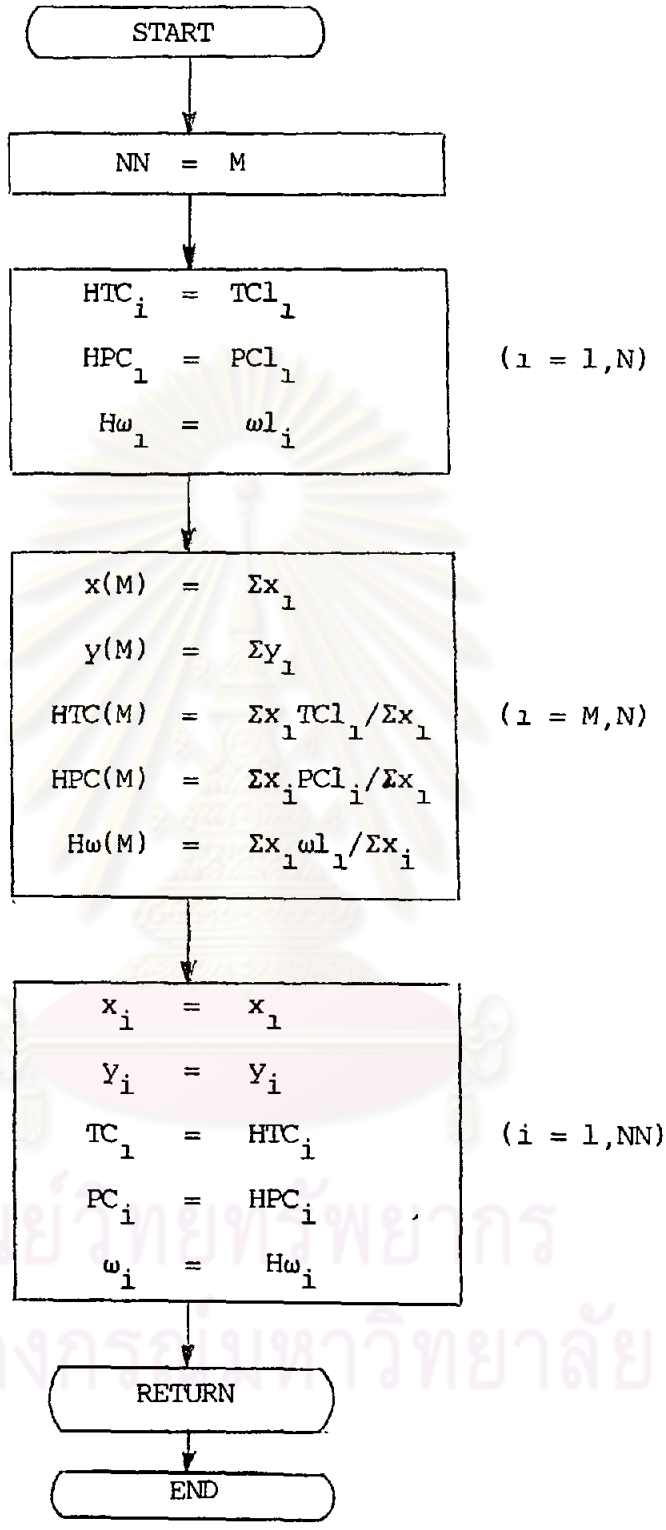

FIGURE 4.6 ALGORITHM FOR GROUPING HEAVY-PSEUDOCOMPONENT

(SUBROUTINE HEAVY)

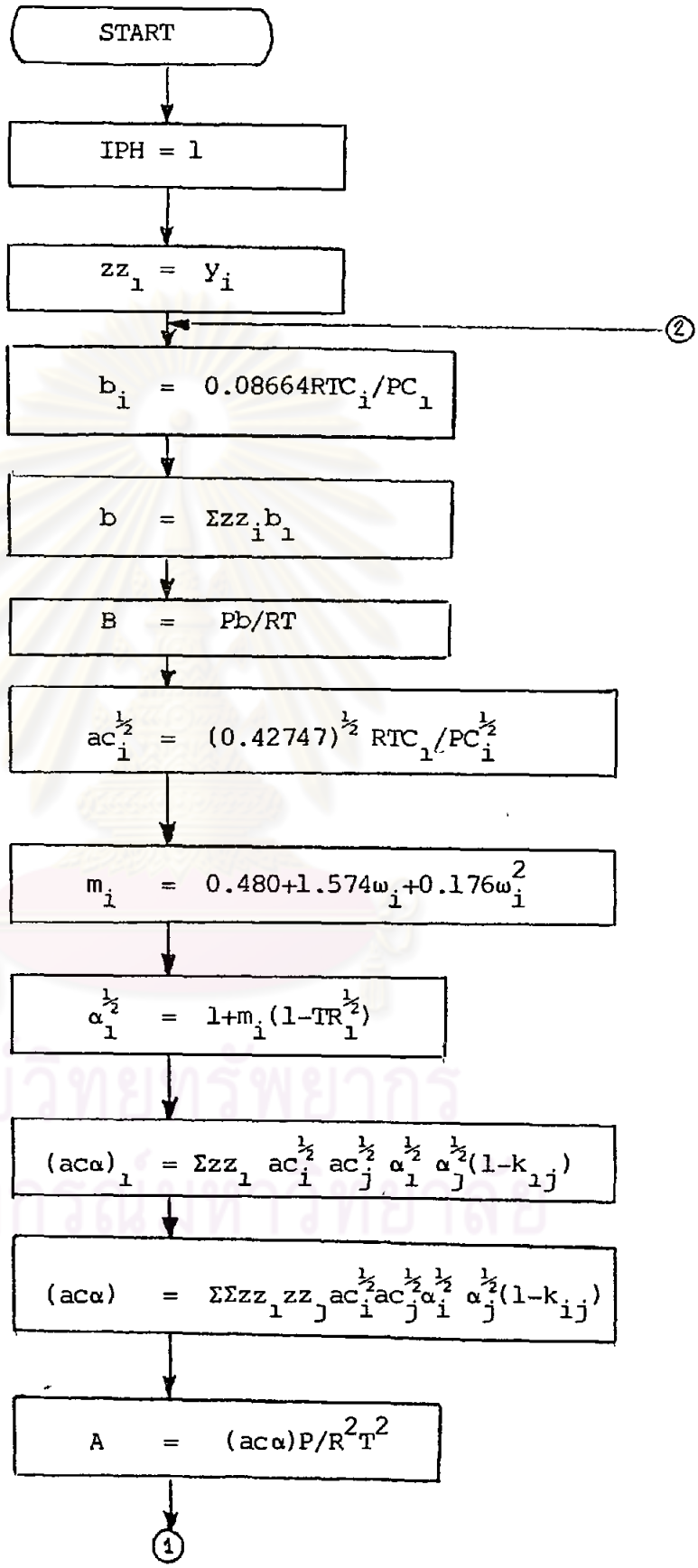

FIGURE 4.7 ALGORITHM OF THE SOAVE-REDLICH-KWONG EQUATION OF STATE

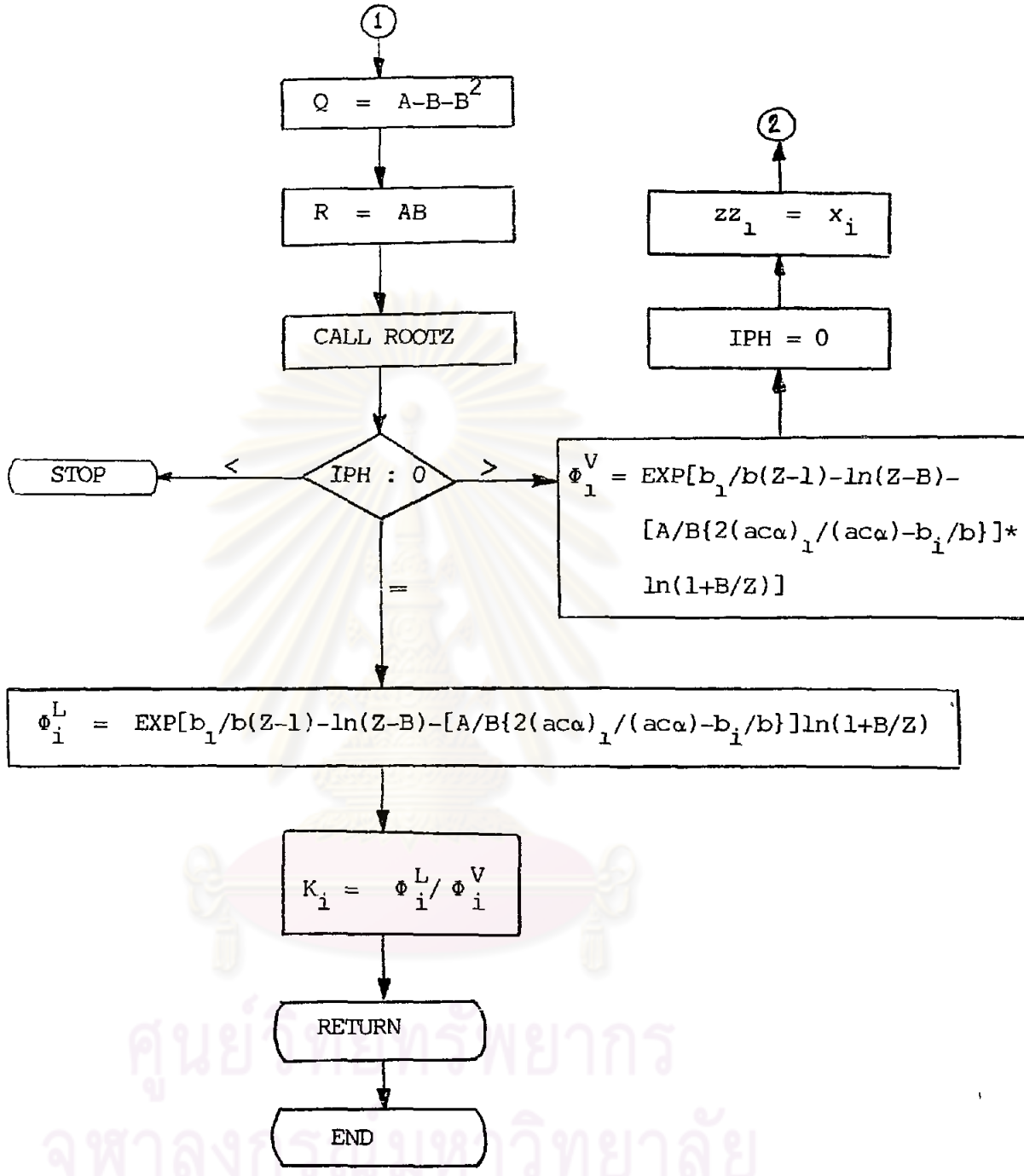

FIGURE 4.7 ALGORITHM OF THE SOAVE-REDLICH-KWONG EQUATION OF STATE (CONTINUED)

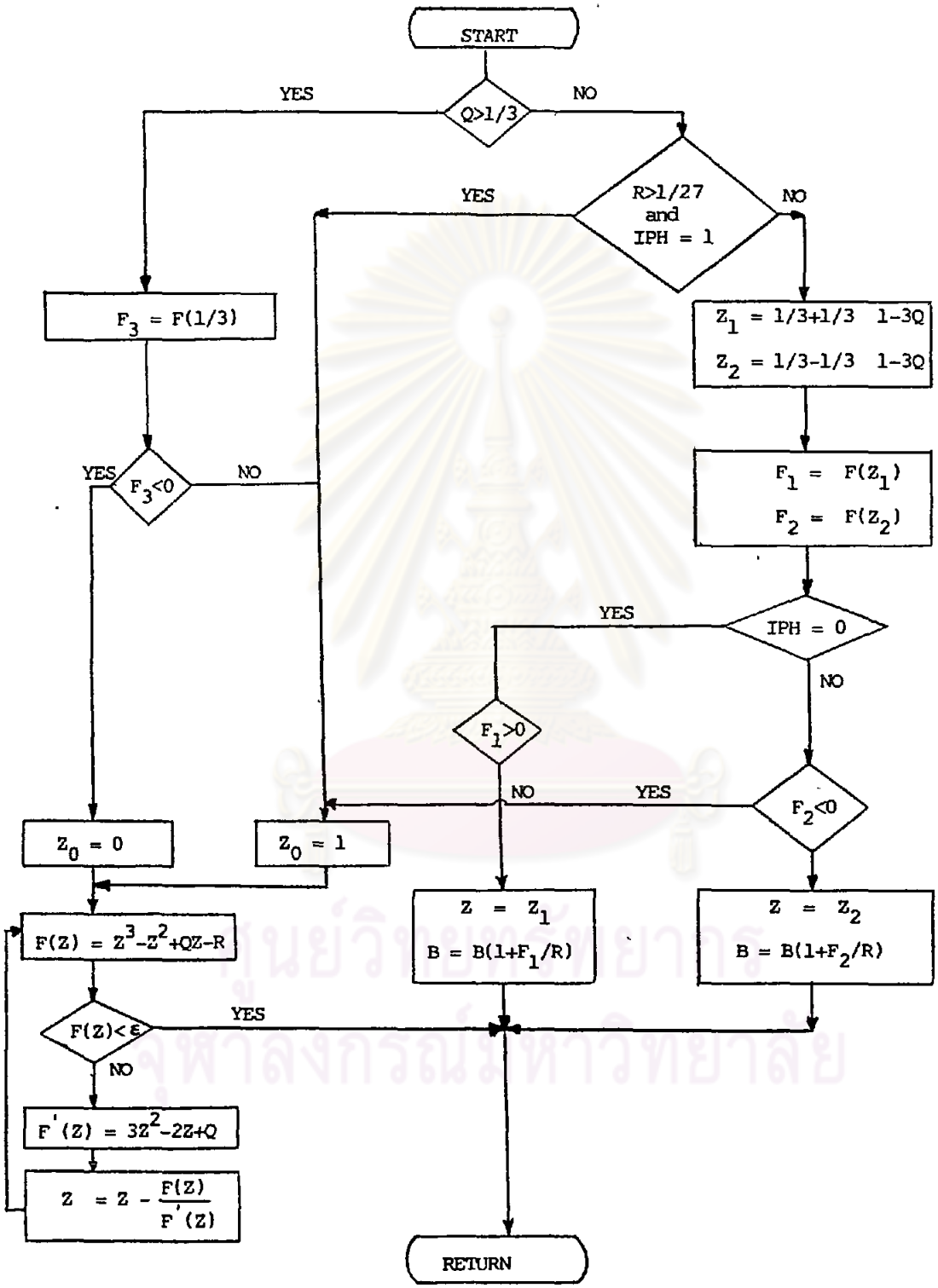

FIGURE 4.8 ALGORITHM FOR THE SOLUTION OF THE CUBIC EQUATION OF STATE (Z-COMPRESSIBILITY FACTOR) (SUBROUTINE ROOTZ)

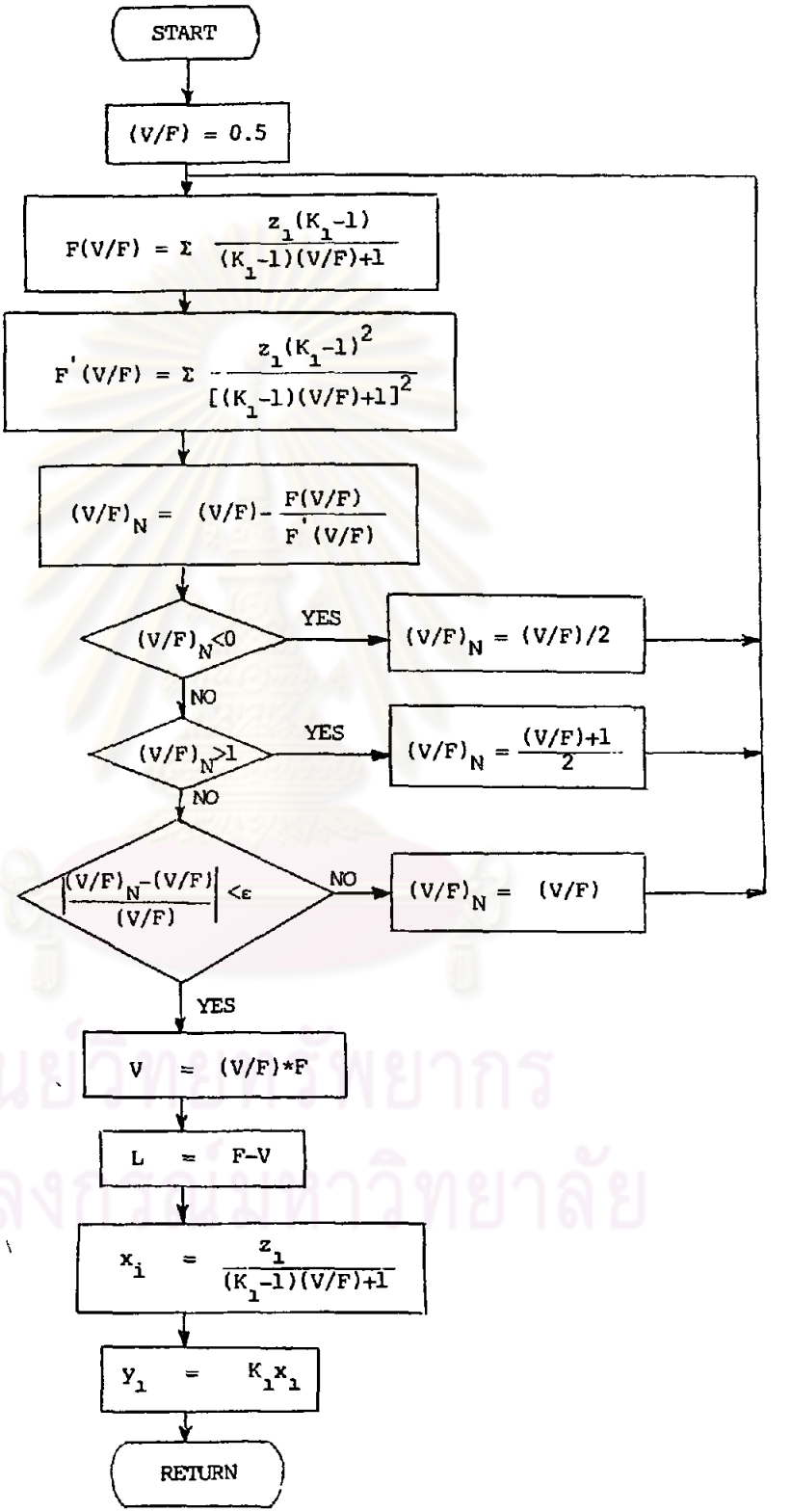

FIGURE 4.9 ALGORITHM OF EQUILIBRIUM FLASH CALCULATION (SUBROUTINE FLASH)

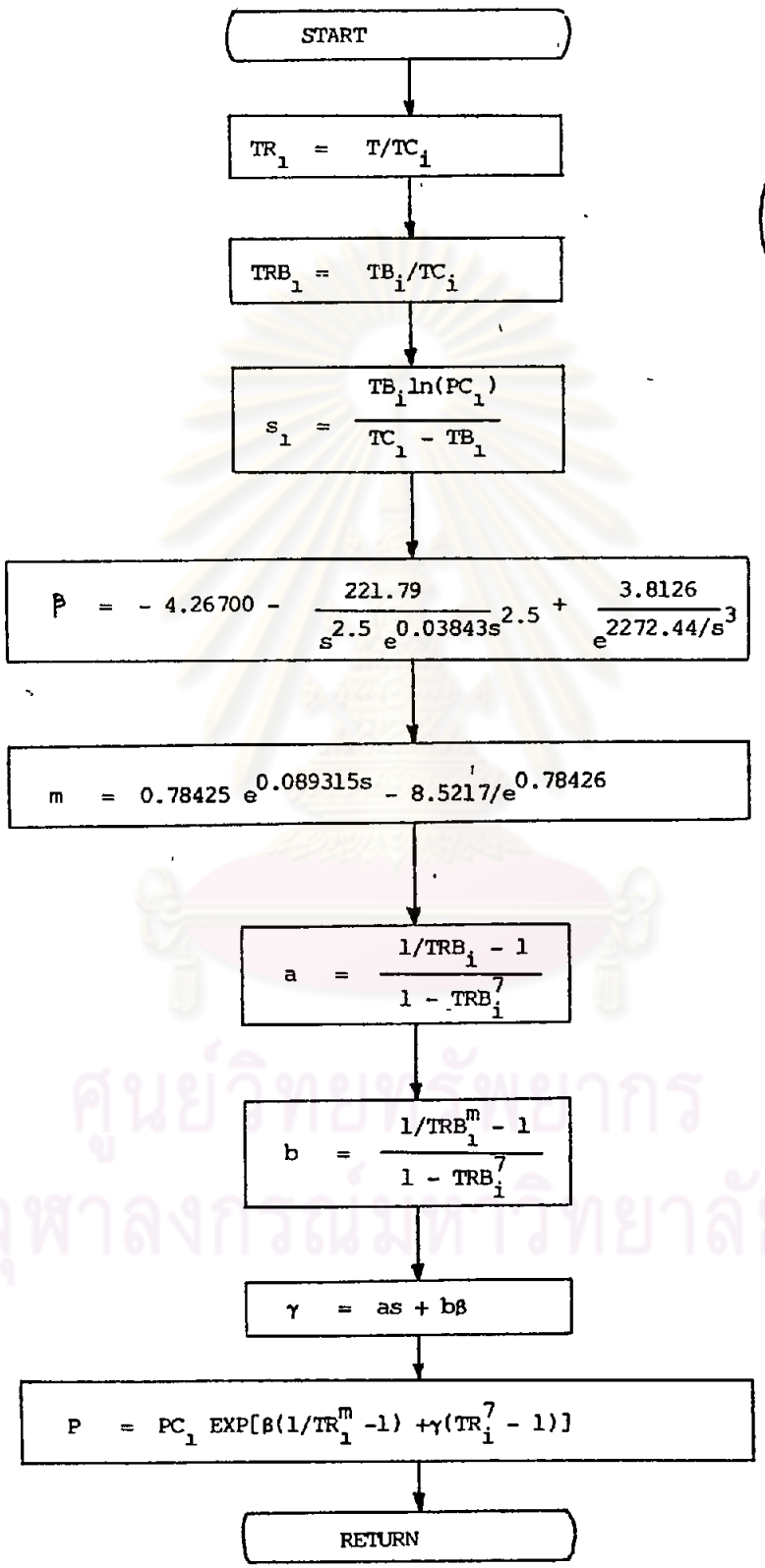

FIGURE 4.10 ALGORITHM OF VAPOR PRESSURE CALCULATION

(see APPENDIX II)

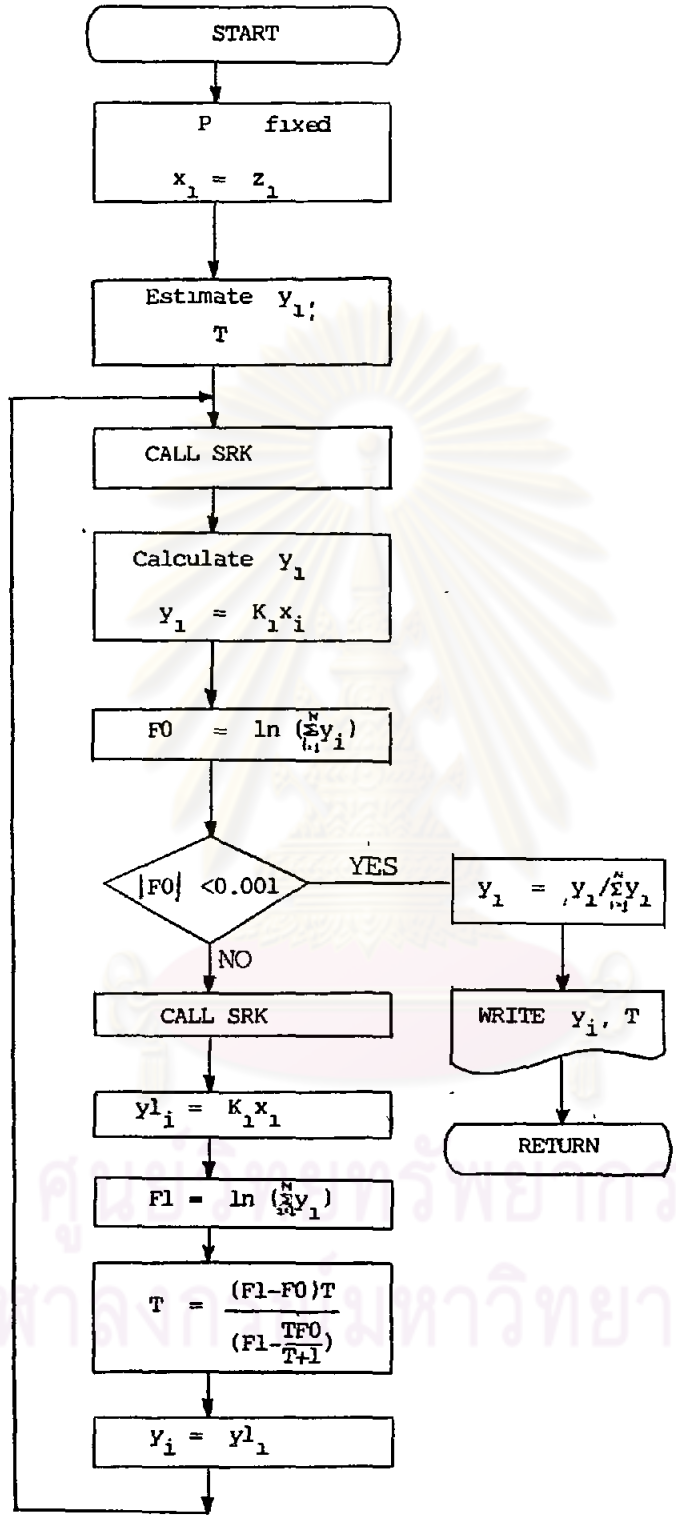

FIGURE 4.11 ALGORITHM OF BUBBLE POINT TEMPERATURE CALCULATION (SUBROUTINE DEWBUB)

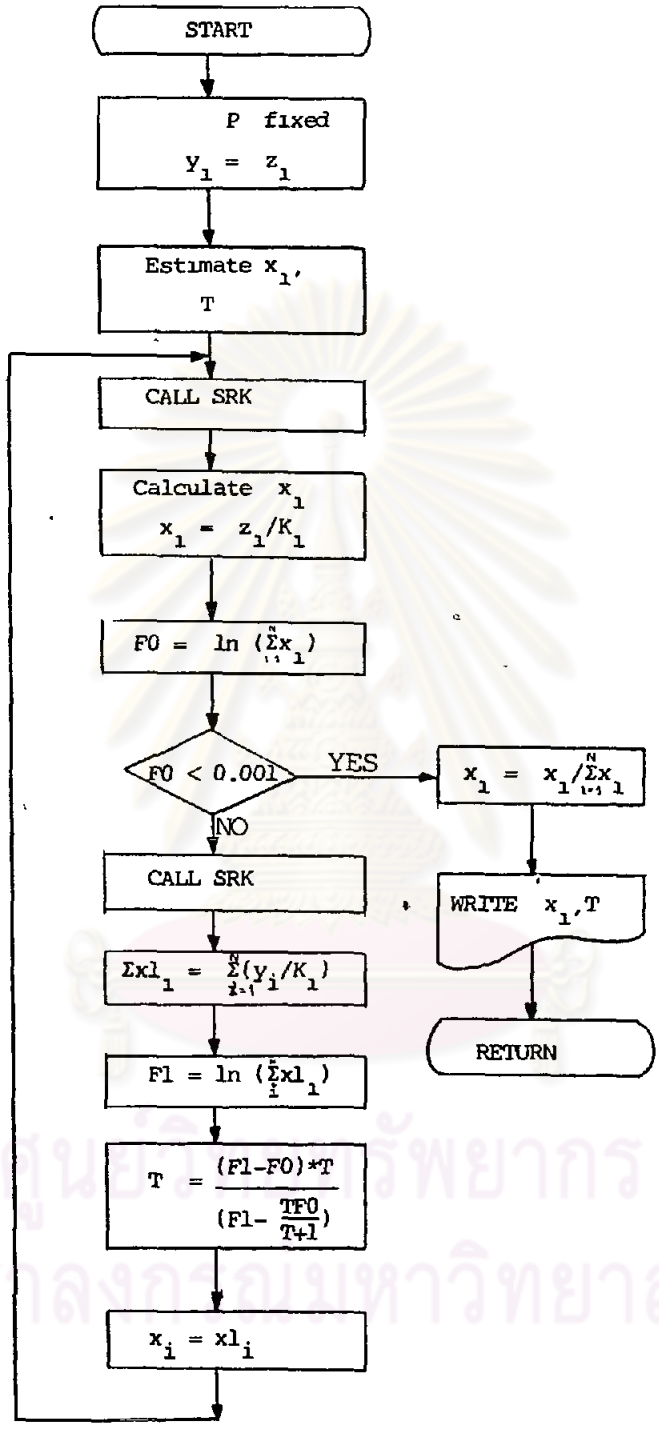

FIGURE 4.12 ALGORITHM OF DEW POINT TEMPERATURE CALCULATION (SUBROUTINE DEWBUB)

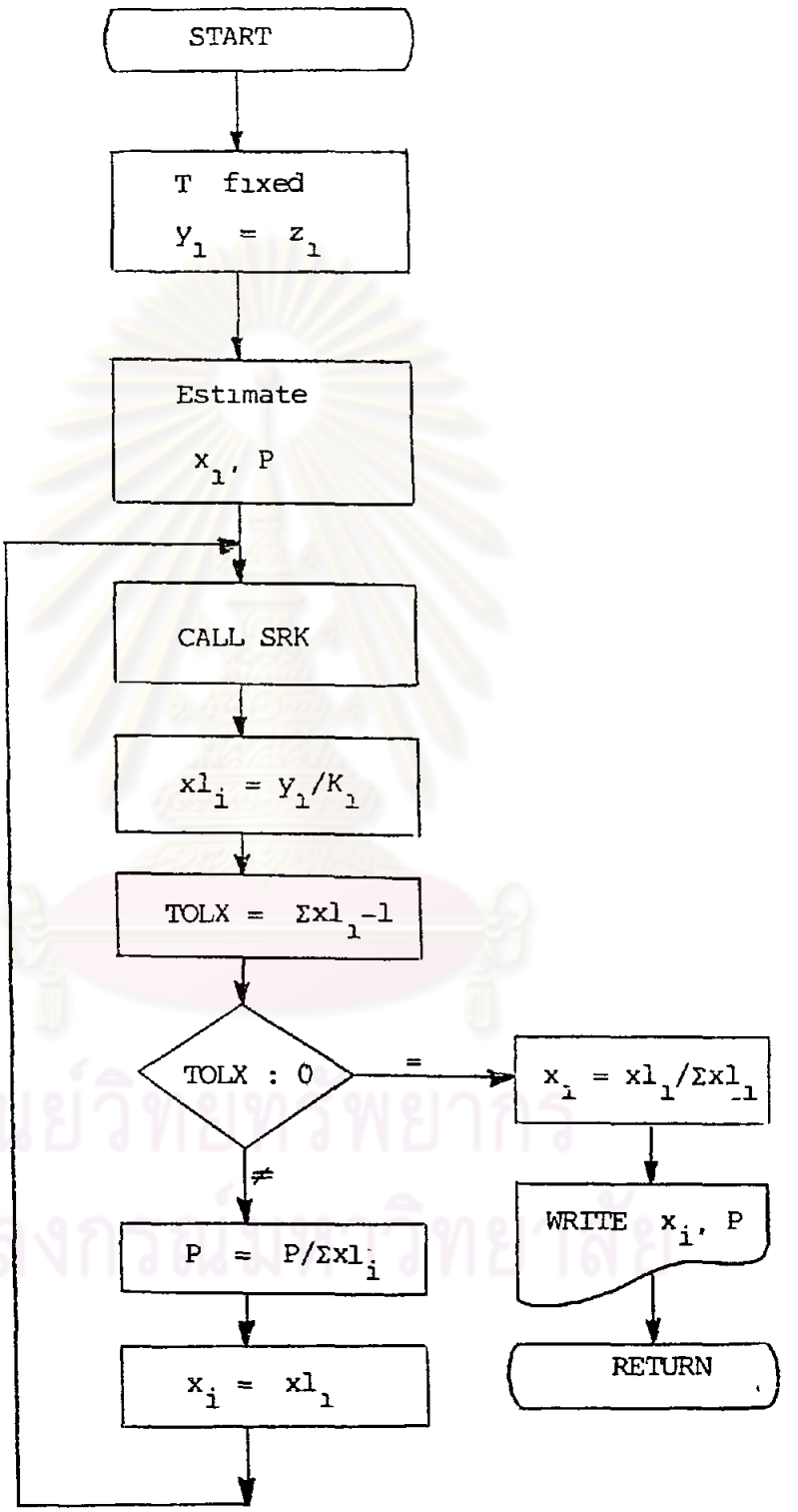

FIGURE 4.13 ALGORITHM OF BUBBLE POINT PRESSURE CALCULATION (SUBROUTINE DEWBUB)

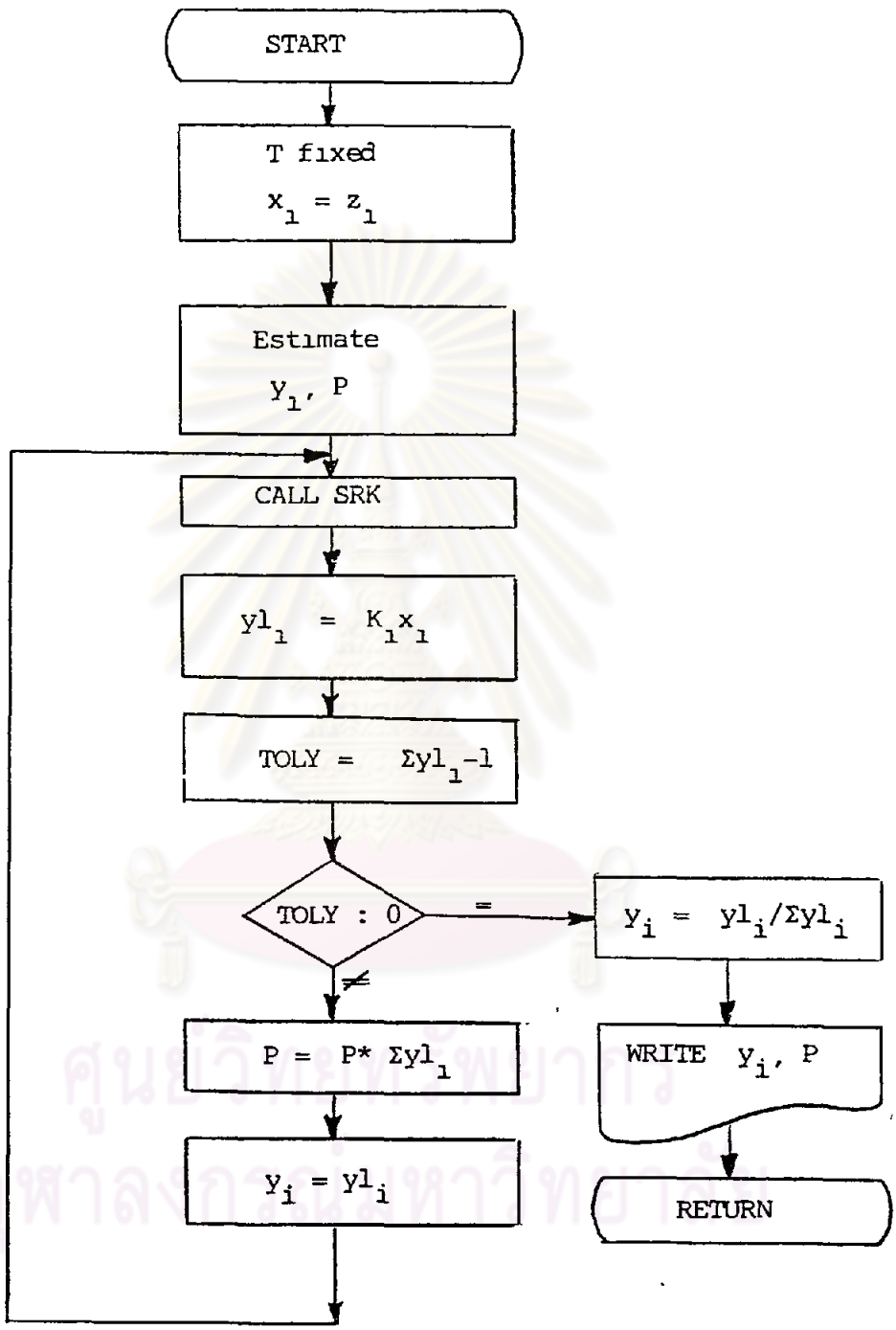

FIGURE 4.14 ALGORITHM OF DEW POINT PRESSURE CALCULATION

(SUBROUTINE DEWBUB)