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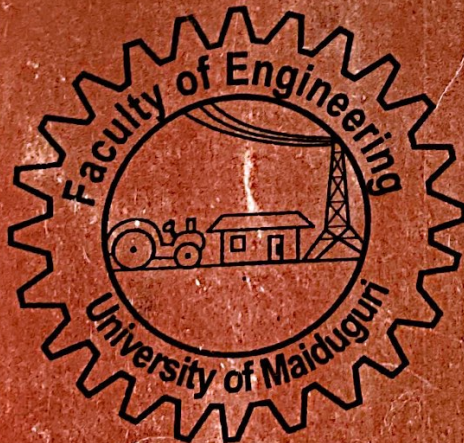
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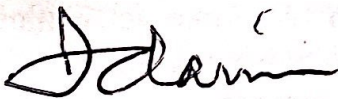
FOREWORD

I am delighted to see another volume of the Faculty of Engineering Seminar Series published. I am particularly happy to note that the staff of the Faculty are very much focused and engaged in research activities that are very relevant not only to us but worldwide.

It is sad to note that over the last few years there was very little fund to support meaningful research activities. This is certainly not a healthy development for a university that has research as one of its main functions. It is our hope that the government will take necessary steps to improve research funding. We also expect private sector funding for university research. The staff are also encouraged to look for external funding for their research to supplement the effort of the university in this regard.

In order to fully utilize the limited resources available to us and to emphasize multidisciplinary approach, the current administration decided to channel all, but a few, research activities in the University of Maiduguri through the four research centres of the University, namely Centre for Biotechnology Research, Centre for Arid Zone Studies, Centre for Trans-Saharan Studies and Centre for Peace and Development Studies. The University has also identified some research themes and sub-themes as the general research focus for implementation by the academic departments towards achieving the required capability and technical development in areas of both Science and Humanities. It is therefore necessary for all staff to have close contact with the research centres to find out where their researches will fit and could be funded. We are providing some money from the internally generated revenue to fund such projects in 2007.

Finally, I congratulate all staff of the Faculty of Engineering for their effort in keeping the seminar series alive.



Professor J.D. Amin, OFR
Vice-Chancellor, University of Maiduguri

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COMPUTER SIMULATION OF SEPARATION UNIT WITH VISUAL USER'S INTERFACE

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ABSTRACT

Separation processes are commonly encountered in all processing industries, which make their design and evaluation very important. Simulation of the separation process presented in this paper was based on successive approximation method which is a unit performance evaluation method yielding the optimal value for a specified unit operating condition. The developed simulation was taken a step further by creating an interactive user friendly interface developed with visual studio C++.

INTRODUCTION

In process industries, apart from when a chemical reaction is involved, commonly mixtures are separated into two or more components. Therefore, separation processes could be defined as those operations which transform a mixture of substances into two or more products differing from one another in composition by addition of a separating agent in the form of matter and/or energy in another stream, as depicted in Fig. 1 (King, 1971).

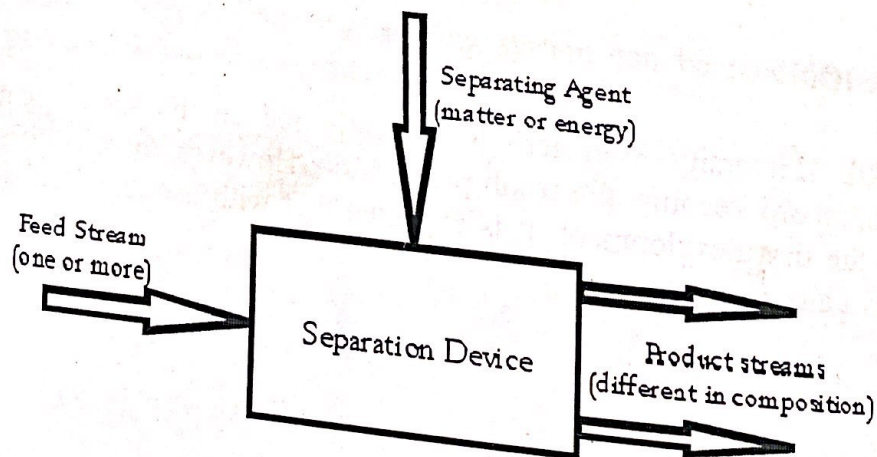


Fig. 1. General separation processes

While the act of modeling of separation units is a routine exercise in process engineering, precise solutions to the models are traditionally handled by the cumbersome manual computation practice with its inherent time consumption and error prone due to human fatigue from a monotonous lengthy task. Unfortunately, accuracy in modeling and analysis can not be ignored, for the result of the modeling determines the size of the separation equipment. In most chemical processes, separation equipment account for about fifty to ninety percent of the capital investment. In fact, separation processes determine very often the cost of the final product (King, 1971).

Digital computation proffers better solution to most of the human limitations enumerated above. Simulation of a separation process and incorporating it into a visual interface readily turn the code into a user friendly computer software, requiring only the supply of some set of independent data, and the software readily performs the required calculations of the stage requirements in multi-component Flashes, Distillation Columns, Extraction Unit, Absorbers, Strippers, etc.

There are three distinctive methods usually employed in the analysis of multi-component multi-stage separation processes, namely stage-to-stage calculation method, group method and successive approximation method. Successive approximation method is preferred because it improves on the limitations of the stage-to-stage and group methods. The successive approximation method is self-starting and does not depend on good prediction of the initial estimates of the reference stage compositions as the stage-to-stage calculation method requires. Also, all stages are considered together within a single iteration of the trial and error procedures unlike the group calculation method that only gives consideration to the feed and product stage composition without considering the intermediate stages (King, 1971).

There are many process design softwares for industrial and educational purposes and all of them incorporate separation unit into the simulation package (Schneider and Marquardt, 2003). The two most common in the academics are Hysys and Aspen process simulators which assist in courses on computer-aided design (Oners and Oners, 2001; Fernandes, 2002). Some institutions developed their own process simulators making use of the good but old McCabe-Thiele and Ponchon-Savarit methods for stage distillation design and graphical methods for gas absorption and stripping design (Oners and Oners, 2001). Most of these process simulator software packages are very expensive. Therefore the computer code and even the logic are not released, but generally reference is always made to separation process text as the basis for their model.

The objective of this paper is to create a foundation for converting most of the chemical engineering design process models to computer software packages, which will invariably lead to indigenous process design software.

Notation

$v_{j,k}$	Moles of component j leaving stage k in vapour phase per time
$l_{j,k}$	Moles of component j leaving stage k in liquid phase per time
$s_{v,j,k}$	Vapour moles of component j in side stream leaving stage k per time
$s_{l,j,k}$	Liquid moles of component j in side stream leaving stage k per time
$f_{v,j,k}$	Vapour moles of component j in feed stream entering stage k per time
$f_{l,j,k}$	Liquid moles of component j in feed stream entering stage k per time
V_k	Total moles of vapour leaving stage k per time
L_k	Total moles of liquid leaving stage k per time
$S_{v,k}$	Total moles of vapour in side stream leaving stage k per time
$S_{l,k}$	Total moles of liquid in side stream leaving stage k per time
$F_{v,k}$	Total moles of vapour in feed stream leaving stage k per time
$F_{l,k}$	Total moles of liquid in feed stream leaving stage k per time
V_0	Total moles of vapour entering unit per time
L_{N+1}	Total moles of liquid entering unit per time
N	Total number of stages
k	Represent a stage k , from 1 to N
j	Represent a component j , from 1 to C
ΔV_{sk}	Vapour summation difference
ΔL_{sk}	Liquid summation difference
H_k	Total specific enthalpy of vapour leaving stage k per time
h_k	Total specific enthalpy of liquid leaving stage k per time
$H_{s,k}$	Total specific enthalpy of vapour in side stream leaving stage k per time
$h_{s,k}$	Total specific enthalpy of liquid in side stream leaving stage k per time
$H_{f,k}$	Total specific enthalpy of vapour in feed stream entering stage k per time
$h_{f,k}$	Total specific enthalpy of liquid in feed stream leaving stage k per time
$K_{f,k}$	Equilibrium constant for component j , at a given temperature and pressure on stage k

METHODOLOGY

The methodology consists of the following:

- Modeling and simulation of a chemical separation process (emphasis on distillation and absorption units) based on successive approximation method.
- Developing an algorithm for the model.
- Computer simulation of multi-component separation processes.
- Incorporating the simulation into a visual interface.

THEORY

The Model

The separation unit modeling diagram under consideration is shown in Fig. 2. This is for a multi-component multi-stage separation process with countercurrent flow of solute and solvent at steady-state conditions with no chemical reaction in the unit. It is also assumed that the system is in equilibrium.

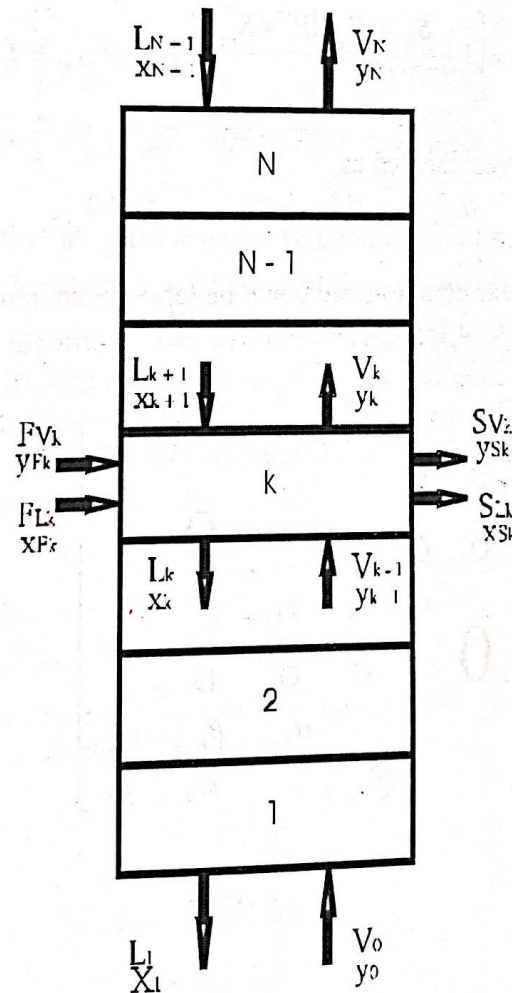


Fig. 2. Separation unit modeling diagram

Successive Approximation Analysis

The material and energy balance on the separation unit yielded the following set of equations (Biegler et al., 1998):

$$L_k = V_{k-1} - V_N + L_{N+1} - \sum_k S_k + \sum_k F_k \quad (1)$$

$$V_k H_k + L_k h_k + S_{vk} H_{sk} + S_{lk} h_{sk} - V_{k-1} H_{k-1} - L_{k+1} h_{k+1} - F_{vk} H_{fk} - F_{lk} h_{fk} = 0 \quad (2)$$

$$v_{j,k} = \frac{K_{j,k} V_k}{L_k} \cdot l_{j,k} \quad (3)$$

$$\sum_j \frac{K_{j,k} V_k}{L_k} \cdot l_{j,k} - V_k = \Delta V_{S_k} \quad (4)$$

$$\sum_j l_{j,k} - L_k = \Delta L_{S_k} \quad (5)$$

$$-\left[\frac{K_{j,k-1} V_{k-1}}{L_{k-1}} \right] \cdot l_{j,k-1} + \left[1 + \frac{S_{lk} + K_{j,k} (V_k + S_{vk})}{L_k} \right] \cdot l_{j,k} - l_{j,k+1} - f_{vj,k} - f_{lj,k} = 0 \quad (6)$$

Equation (6) can be represented as,

$$\alpha_k l_{j,k-1} + \beta_k l_{j,k} + \gamma_k l_{j,k+1} + \varphi_k = 0 \quad (7)$$

Equation (7) is a linear equation and could be represented in matrix form as:

$$\underline{A}_j(t) \cdot \underline{x}_j(t) = \underline{v}_j(t) \quad (8)$$

where

$$\underline{A}_j(t) = \begin{bmatrix} \beta_1 & \gamma_1 & & & \\ \alpha_2 & \beta_2 & \gamma_2 & & \\ & 0 & 0 & 0 & 0 \\ & & \alpha_k & \beta_k & \gamma_k \\ 0 & & 0 & 0 & 0 \\ & & & \alpha_{N-1} & \beta_{N-1} & \gamma_{N-1} \\ & & & & \alpha_N & \beta_N \end{bmatrix} \quad (9)$$

$$\underline{x}_j(t) = \begin{bmatrix} l_{j,1} \\ l_{j,2} \\ M \\ l_{j,k} \\ M \\ l_{j,N-1} \\ l_{j,N} \end{bmatrix} \quad (10)$$

$$\underline{v}_j(t) = \begin{bmatrix} \varphi_1 \\ \varphi_2 \\ M \\ \varphi_k \\ M \\ \varphi_{N-1} \\ \varphi_N \end{bmatrix} \quad (11)$$

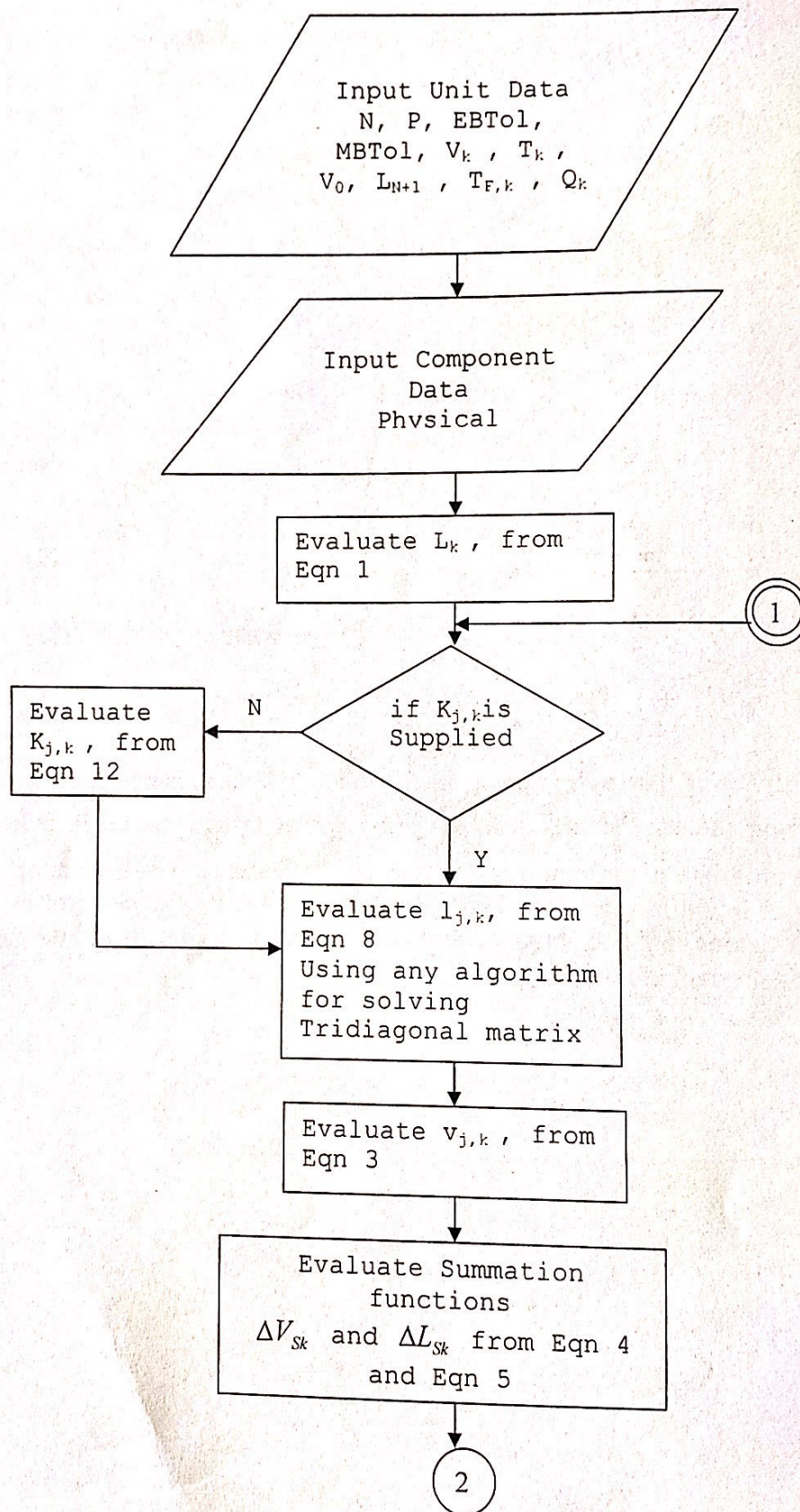
$$K_j = \frac{P_j^o}{P_T} \quad (12)$$

$$\Delta H_v^j = \Delta H_{fj}^o + \int_{T^o}^T C_{p_j}^o(T) dT \quad \text{per mole} \quad (13)$$

$$\Delta H_L^j = \Delta H_{fj}^o + \int_{T^o}^T C_{p_j}^o(T) dT - \Delta H_{vap}^j(T) \quad \text{per mole} \quad (14)$$

It is worth noting that φ_k represents the summation of all streams either vapour or liquid entering stage k. Matrix $A_j(t)$ is a tri-diagonal matrix and could be solved using an appropriate algorithm. The solution of this linear algebraic equation gives the amount of liquid leaving each stage in the separation unit, and the corresponding equilibrium vapour could be obtained from Eqn (3). For model details and derivations of equations one can refer to King (1971) and Oladokun (2003).

Successive Approximation Flow-chart



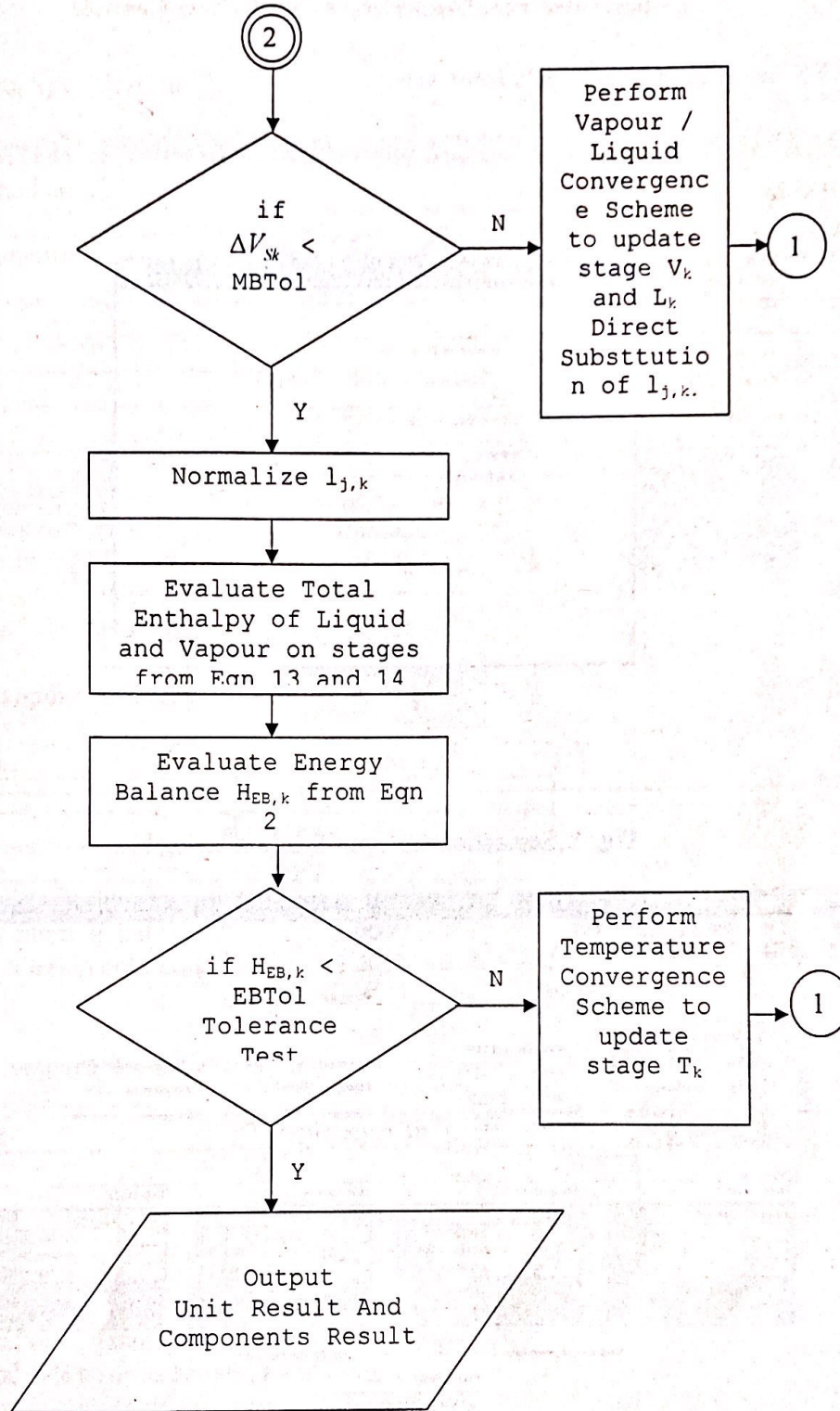


Fig. 3. Separation unit simulation flow-chart

ARK Separation Unit User's Interface

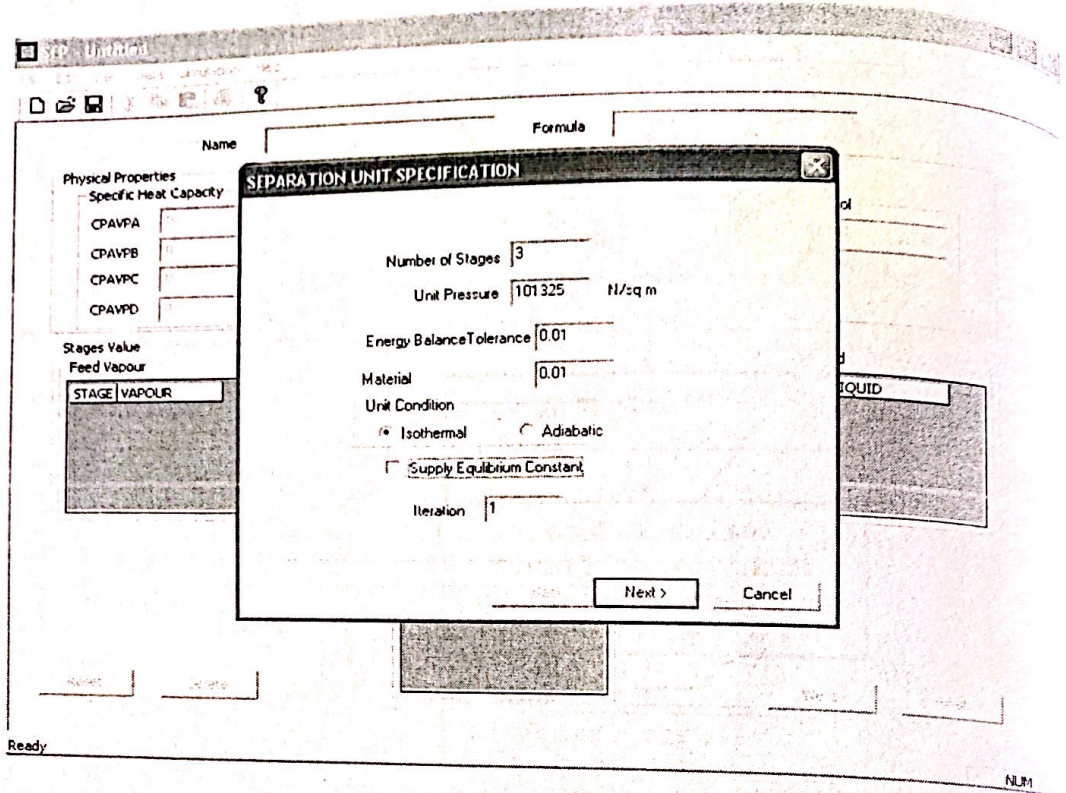


Fig. 4. Separation unit specifications dialog box

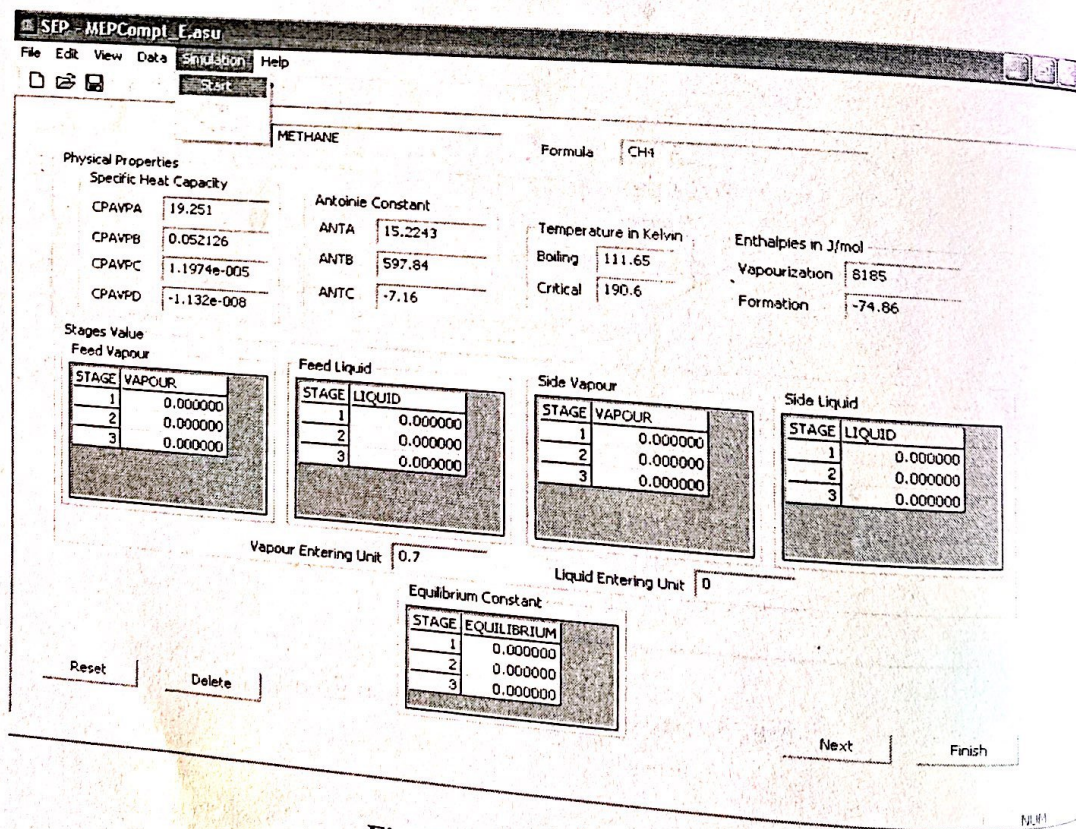


Fig. 5. Simulation process

Problem Specification

A mixture of hydrocarbon with the compositions stated below was fed into an absorption unit:

Components	Amount in Gas Entering Unit (V_0)	Amount in oil Entering the Unit. (L_{N+1})
C ₁	0.7	-
C ₂	0.2	-
C ₃	0.1	-
Oil	-	3.0
	1.0	3.0

Number of stages: 3
 Unit operating pressure: 101325 N/m²
 Energy balance tolerance: 0.01
 Material balance tolerance: 0.01

Initial vapour estimates V_k

Stage k	Vapour Amount, V_k
1	0.9583
2	0.9183
3	0.8800

Vapour entering unit, V_0 : 1.0000
 Liquid entering unit, L_{mN+1} : 3.0000

Initial temperature estimates T_k

Stage k	Temperature in °C	Temperature in K
1	35.75	308.75
2	33.75	306.75
3	31.84	304.84

Temperature of liquid entering unit, T_{N+1} : 30 °C = 303 K
 Feed and side streams temperature equals Zero.
 Feed and side streams amount equal Zero.
 Heat was not added or removed from any stage.

RESULTS AND DISCUSSION

The above specified problem converges after two iterations with the results for both iterations for each component vapour and liquid compositions leaving each stage (Tables 1-3, Fig. 6-11).

Methane

Table 1. Methane vapour and liquid compositions leaving each stage

Methane				
Stage Number	1 st Iteration		2 nd Iteration	
	Vapour	Liquid	Vapour	Liquid
1	0.700133756	0.003074151	0.700055273	0.002869067
2	0.700256533	0.003207907	0.700201061	0.002924340
3	0.696925849	0.003330684	0.697130933	0.003070129

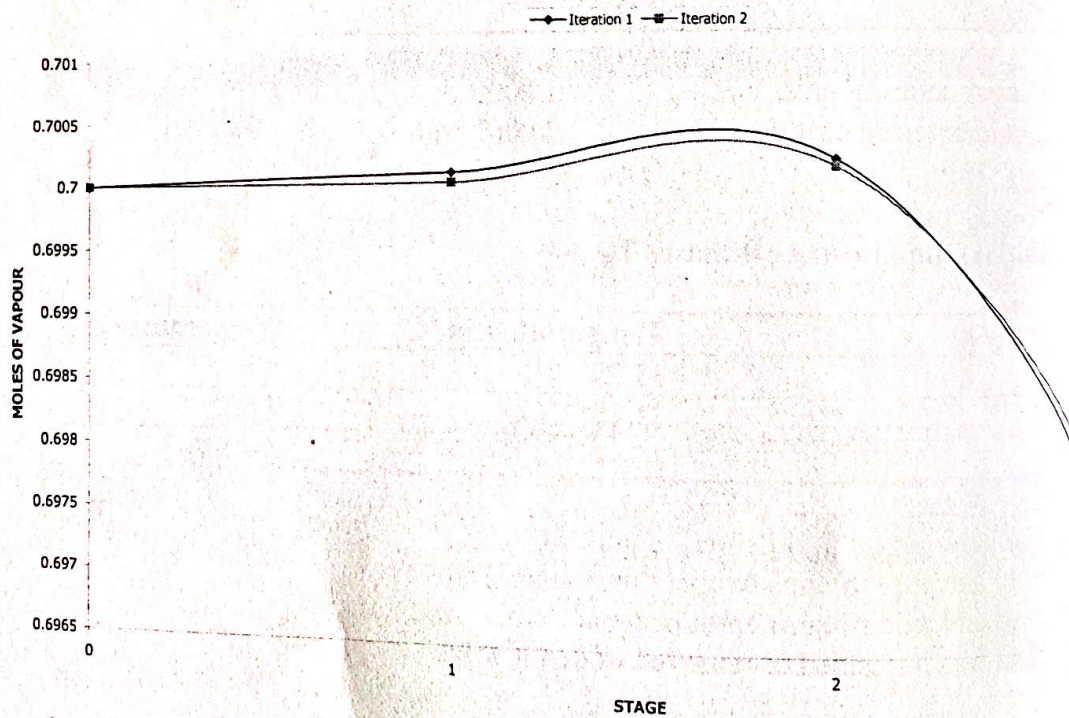


Fig. 6. Variation of methane vapour leaving each stage per iteration

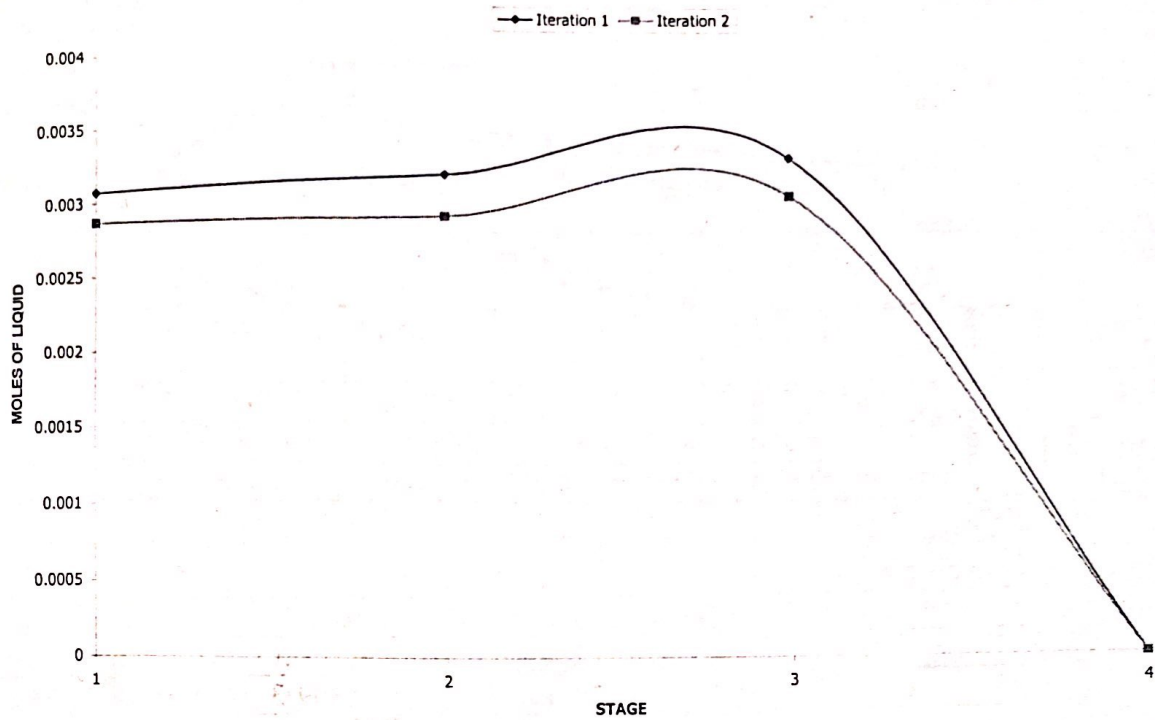


Fig. 7. Variation of methane liquid leaving each stage per iteration

From the second iteration result (Table 1), the amount of methane absorbed in the unit was 0.002869067 moles which represent 0.41% of the fed methane (0.7 moles). As expected, there was a trace amount of methane.

Ethane

Table 2. Ethane vapour and liquid compositions leaving each stage

Ethane					
Stage Number	1 st Iteration		2 nd Iteration		
	Vapour	Liquid	Vapour	Liquid	
1	0.200924303	0.013962369	0.200554562	0.013008385	
2	0.200747821	0.014886671	0.2006165664	0.013562947	
3	0.186037631	0.014710189	0.186991615	0.013624949	

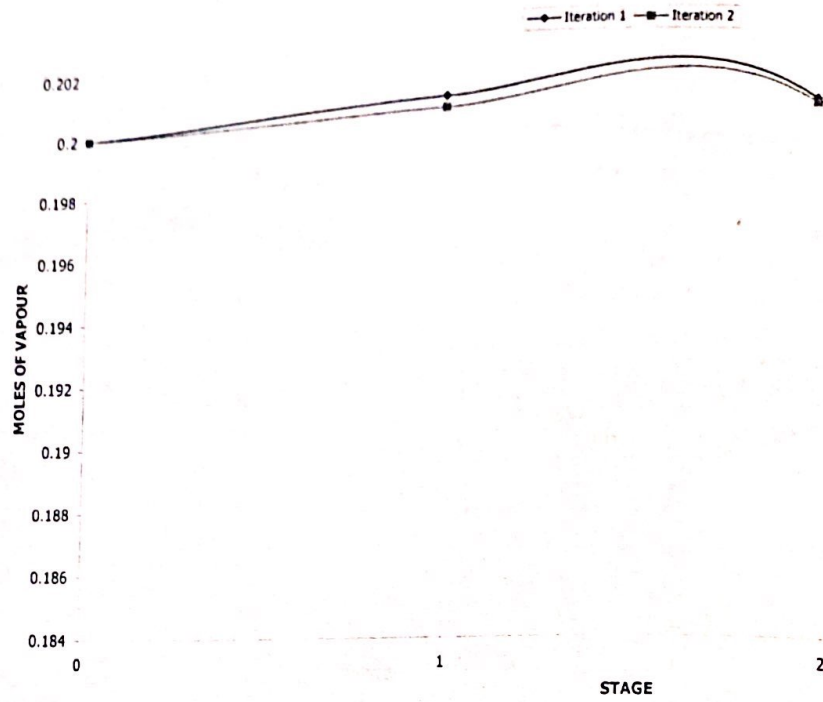


Fig. 8. Variation of ethane vapour leaving each stage per iteration

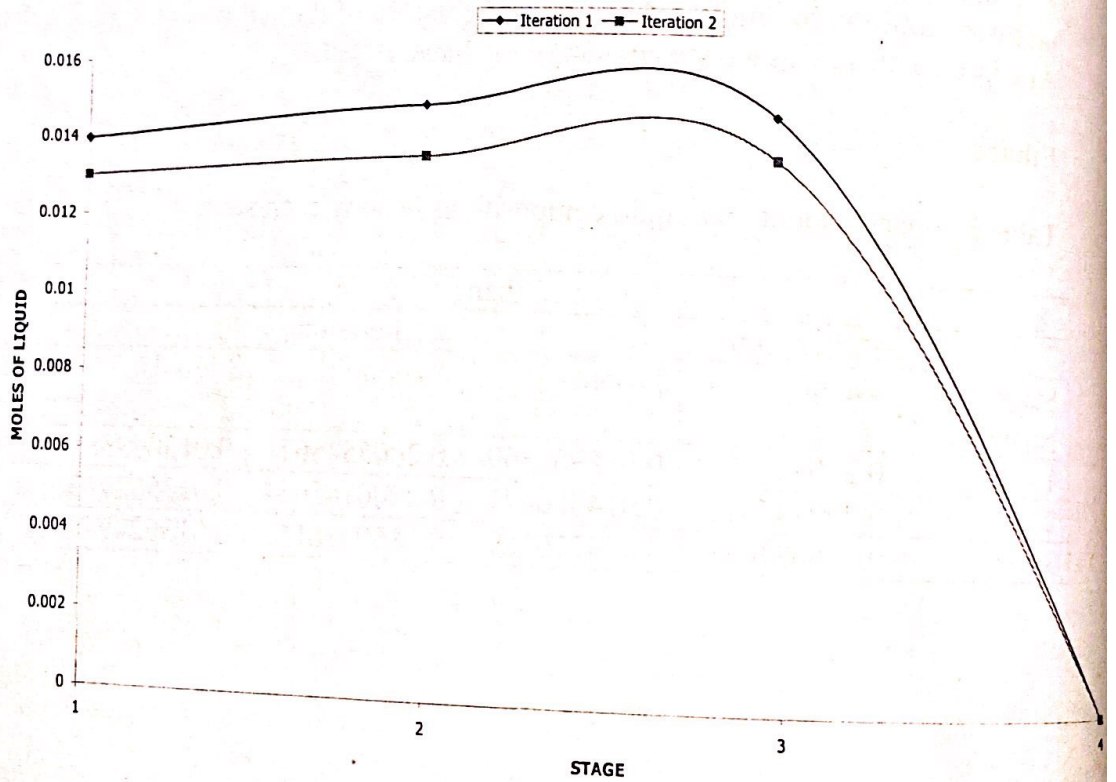


Fig. 9. Variation of ethane liquid leaving each stage per iteration

Similarly, from the second iteration result (Table 2), the amount of ethane absorbed in the unit was 0.013008385 moles which represent 6.5% of the fed ethane (0.2 moles).

Propane

Table 3. Propane vapour and liquid compositions leaving each stage

Propane					
Stage Number	1 st Iteration		2 nd Iteration		
	Vapour	Liquid	Vapour	Liquid	
1	0.100689570	0.027180693	0.100310053	0.025274624	
2	0.095680879	0.027870262	0.096343747	0.025584677	
3	0.072819307	0.022861572	0.074725376	0.021618371	

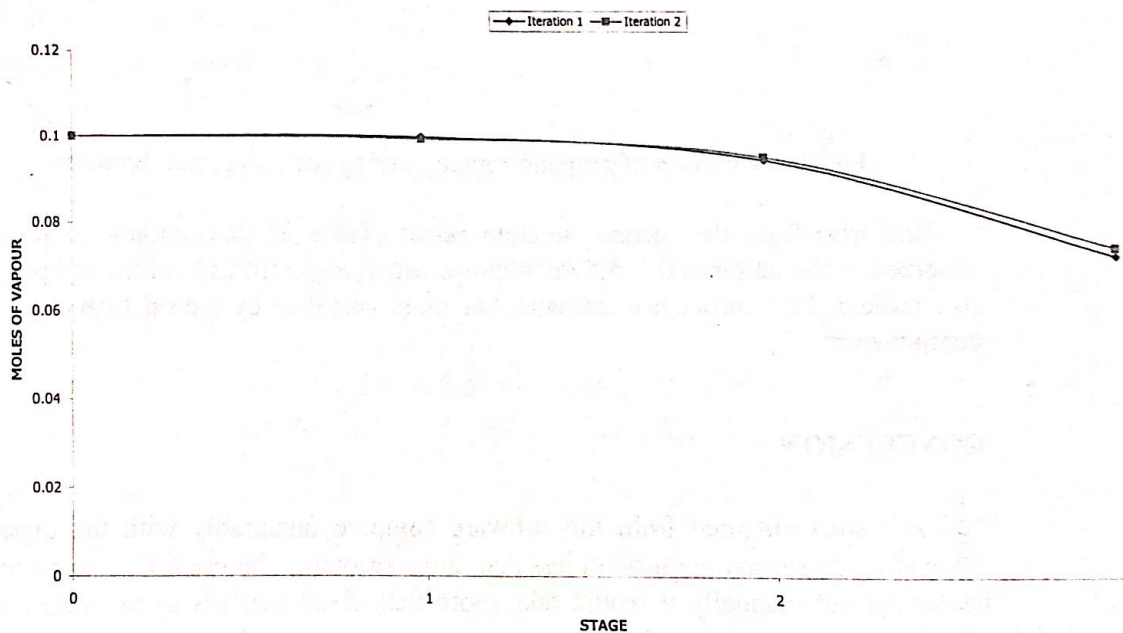


Fig. 10. Variation of propane vapour leaving each stage per iteration

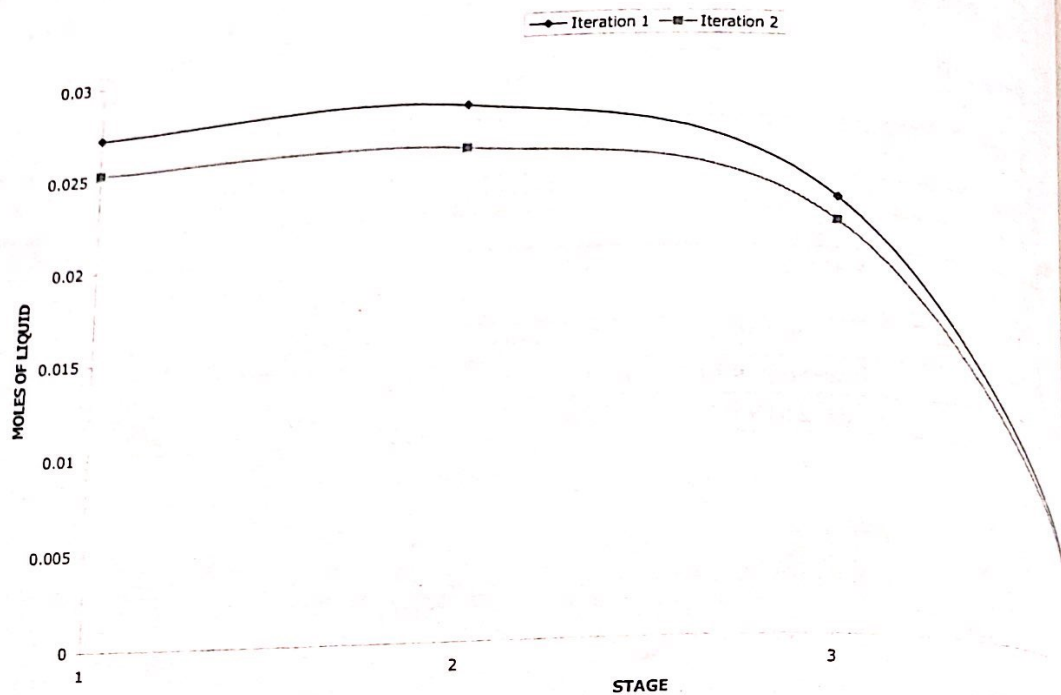


Fig. 11. Variation of propane vapour leaving each stage per iteration

Similarly, from the second iteration result (Table 3), the amount of propane absorbed in the unit was 0.025274624 moles which represent 25% of the fed propane (0.1 moles). This shows that propane was more absorbed by the oil than any other components.

CONCLUSION

The results obtained from the software compare favourably with the expected value after the second iteration in less than three seconds, whereas for the same test to be carried out manually it would take more than three hours with possible human error.

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