

การสร้างแบบจำลองทางคอมพิวเตอร์และทำอุปกรณ์ในเชิง  
ของหอกลั่นหลักที่มีอยู่ในโรงกลั่นน้ำมัน



นายพลชม จันทร์อุไร

วิทยานิพนธ์นี้เป็นส่วนหนึ่งของการศึกษาตามหลักสูตรปริญญาวิศวกรรมศาสตรมหาบัณฑิต

ภาควิชาวิศวกรรมเคมี

บัณฑิตวิทยาลัย จุฬาลงกรณ์มหาวิทยาลัย

พ.ศ. 2529

ISBN 974-566-881-8

013538

I16639258

COMPUTER MODELLING AND OPTIMIZATION  
OF AN EXISTING OIL REFINERY TOPPING COLUMN

Mr. Polshom Chan-urai

A Thesis Submitted in Partial Fulfilment of the Requirements  
for the Degree of Master of Engineering  
Department of Chemical Engineering  
Graduate School  
Chulalongkorn University  
1986

ISBN 974-566-881-8

Thesis Title      Computer Modelling and Optimization of An Existing  
                      Oil Refinery Topping Column  
By                  Mr. Polshom Chan-urai  
Department        Chemical Engineering  
Thesis Advisor     Associate Professor Wiwut Tanthapanichakoon, Ph.D.

---

Accepted by the Graduate School, Chulalongkorn University in  
Partial Fulfilment of the Requirements for the Master's Degree.

S. Rhi. IL ..... Dean of Graduate School  
(Associate Professor Sorachai Bhisalbutra)  
Acting Associate Dean for Academic Affairs  
for  
Acting Dean of the Graduate School



Thesis Committee

Chairit Satayaprasert ..... Chairman  
(Assistant Professor Chairit Satayaprasert)

Sutham Vanichaseni ..... Member  
(Associate Professor Sutham Vanichaseni)

K. Kroekchai Sukanjanatee ..... Member  
(Associate Professor Kroekchai Sukanjanatee)

Wiwut Tanthapanichakoon ..... Member  
(Associate Professor Wiwut Tanthapanichakoon)

Copyright of the Graduate School, Chulalongkorn University

หัวข้อวิทยานิพนธ์

การสร้างแบบจำลองทางคอมพิวเตอร์และทำอوبติไม้เขียนของหอกลั่นหลักที่มีอยู่ในโรงกลั่นน้ำมัน

ชื่อนิสิต

นายพลชม จันทร์อุไร

อาจารย์ที่ปรึกษา

รองศาสตราจารย์ ดร.วิวัฒน์ ตันตะพาณิชกุล

ภาควิชา

วิศวกรรมเคมี

ปีการศึกษา

2528



บทคัดย่อ

แบบจำลองของหอกลั่นน้ำมันดินที่มีจริงแห่งหนึ่งได้ถูกสร้างขึ้นโดยใช้แนวความคิดของการกลั่นสารผลสมเทียมแฟรงหลายชนิด (pseudomulticomponent) น้ำมันดินจะถูกแบ่งเป็นส่วนประกอบ (fractions) ที่มีคุณสมบัติต่างกันซึ่งจำนวน 39 ส่วน ในขั้นตอนแรกได้ทำการกำหนดหอคุปمان เอิงทฤษฎี (theoretical analogue) ของหอกลั่นจริง ปรากฏว่าผลการคำนวณของหอกลั่นอุปมานนี้ สอดคล้องอย่างดีพอควรกับข้อมูลที่ได้จากหอกลั่นจริง รวมทั้งอุณหภูมิของแต่ละชั้นและเส้นแสดงจุดเดือดจริงของการกลั่นของทุก ๆ ผลิตภัณฑ์แยกได้ วิธีที่ใช้แก้แบบจำลองได้ปรับปรุงมาจากวิธีของนิวตัน-ราฟลัน ต่อไป ได้ใช้โปรแกรมคอมพิวเตอร์นี้ จำลองผลการกลั่นน้ำมันดินที่สภาวะอัตราส่วนการป้อนกลับและอุณหภูมิการแฟลชต่าง ๆ และเปรียบเทียบเงื่อนไขการทำงานทั้งหมดที่ไม่ได้ให้ผลิตภัณฑ์พิครายละเอียดคุณภาพ เพื่อหาเงื่อนไขการทำงานที่เหมาะสมที่สุดในแต่การเพิ่มกำไรวรุ่ม

จุฬาลงกรณ์มหาวิทยาลัย

Thesis Title      Computer Modelling and Optimization of An Existing  
 Oil Refinery Topping Column  
 Name                Mr. Polshom Chan-urai  
 Thesis Advisor     Associate Professor Wiwut Tanthapanichakoon  
 Department        Chemical Engineering  
 Academic Year     1985



#### ABSTRACT

An actual topping column has been modeled using the concept of pseudomulticomponent distillation. The crude oil is divided into 39 fractions of distinct properties. A theoretical analogue of the actual column is first determined. The simulated results of the analogue column are found to agree reasonably well with the actual data, including the plate temperatures and the TBP distillation curves of the fractionated products. The modified 2N-Newton-Raphson method is used in the simulation. Next the present computer program was used to simulate the crude distillation at various reflux ratio and flash temperatures. Then all operating conditions that did not yield off-specification products were compared to find an optimum condition that most improved the overall profit.

ACKNOWLEDGEMENTS



The author wishes to express his sincere appreciation to Associate Professor Wiwut Tanthapanichakoon for his invaluable advice and comments to this study. Thanks also to Associate Professor Sutham Vanichseni, Assistant Professor Chairit Satayaprasert, and Associate Professor Kroekchai Sukanjanatee for serving on the thesis committee. In particular the author wishes to thank to the Thai Government for the financial support. Finally, the author is indebted to her parents for their encouragements.

Polshom Chan-urai

May, 1986.

ศูนย์วิทยทรัพยากร  
จุฬาลงกรณ์มหาวิทยาลัย



## TABLE OF CONTENTS

	Page
ABSTRACT IN THAI .....	iv
ABSTRACT IN ENGLISH .....	v
ACKNOWLEDGEMENTS .....	vi
TABLE OF CONTENTS .....	vii
LIST OF TABLES .....	x
LIST OF FIGURES .....	xii
NOMENCLATURES .....	xv
 CHAPTER	
1. INTRODUCTION .....	1
2. SURVEY OF THE LITERATURE .....	4
2.1 Rigorous Solutions of Multicomponent Distillation Problem .....	4
2.2 Solutions of Crude Distillation Problem .....	8
3. BASIC KNOWLEDGE IN CRUDE OIL AND ITS FRACTIONATING SYSTEM .....	13
3.1 Characterization of Crude Oil and Its Fractions .....	13
3.1.1 ASTM Distillations .....	13
3.1.2 TBP Distillations .....	18
3.1.3 EFV Distillations .....	21
3.1.4 Interrelation between ASTM, TBP and EFV Distillation Curves .....	21
3.1.5 API Gravity .....	26
3.1.6 UOP Characterization Factor .....	26
3.1.7 Crude Assay .....	28

3.2 Crude Oil Refinery Distillation .....	31
3.2.1 Basic Processes for Topping Column .....	34
3.2.2 Products of Topping Column .....	36
4. MATHEMATICAL MODEL .....	38
4.1 Crude Oil and Petroleum Fraction Models .....	38
4.1.1 Number and Quantities of Components .....	39
4.1.2 Density and Specific Gravity .....	40
4.1.3 Molecular Weight .....	42
4.1.4 Vapor-liquid Equilibrium, K-values .....	48
4.1.5 Vapor and Liquid Enthalpies .....	60
4.2 Topping Column Models .....	72
4.2.1 Choice of Independent Variables .....	75
4.2.2 Total Material Balances .....	76
4.2.3 Component Material Balances .....	79
4.2.4 Component Material Balances for Water .....	82
4.2.5 Corresponding Set of Independent Functions .....	84
4.2.6 Algorithm for Independent Function Evaluation .....	87
5. NUMERICAL SOLUTION OF THE TOPPING COLUMN MODELS .....	88
5.1 Modified Newton-Raphson Method with Broyden-Householder Formula .....	89
5.2 Algorithm of Developed Computer Program .....	91
5.3 Testing the Computer Program on a Known Problem .....	92
6. SIMULATION OF AN EXISTING TOPPING COLUMN .....	104
6.1 Crude and Sidestream Products Models .....	104
6.2 Topping Column Model .....	108
6.3 The Theoretical Analogue Column .....	114

7.	OPIMIZATION OF AN EXISTING TOPPING COLUMN .....	122
7.1	Choice of Operating Variables and Objective of Optimization .....	123
7.2	Product Specifications .....	124
7.3	Summary of Simulation Results .....	126
7.4	Optimization Results .....	126
8.	CONCLUSIONS .....	151
	REFERENCES .....	153
	APPENDICES .....	160
	APPENDIX A. Relation between lb/gal, specific gravity and °API .....	161
	APPENDIX B. Computer Program Output of an Existing Topping Column Simulation .....	166
	APPENDIX C. Flowchart of the Simulation Program .....	185

## LIST OF TABLES

	Page
Table 1 Hydrocarbon analysis of a representative crude - Tia Juana Light .....	14
Table 2 Laboratory Distillation Tests .....	16
Table 3 Properties of representative crude - Arabian Crudes ....	30
Table 4 Boiling Ranges of Typical Crude Oil Fractions .....	37
Table 5 TBP Cut Points for Various Crude Oil Fractions .....	37
Table 6 Composition of the feed stream and other specifica- tions for the theoretical analogue column shown in Fig. 26 .....	96
Table 7 Elements of matrices for total material balances .....	98
Table 8 Elements of matrices for component material balances ....	99
Table 9 Nonzero values of the coefficients of the generalized enthalpy-balance function (Eqs. 60-62) .....	100
Table 10 Initial and final column profiles obtained by the pre- sent computer program and published by Hess et al. ....	101
Table 11 Light-component analysis for the crude oil feed .....	106
Table 12 Pseudocomponents representation of crude oil feed ....	109
Table 13 Vapor-liquid equilibrium data for the pseudocomponents in Table 12 .....	110
Table 14 Liquid enthalpies for the pseudocomponents in Table 12..	111
Table 15 Vapor enthalpies for the pseudocomponents in Table 12...	112
Table 16 ASTM distillation analysis and molal flow rate of the sidestream products .....	113
Table 17 Some of the simulation results at various stage number..	115
Table 18 Initial and final values compared .....	116

	Page
Table 23 Summary of thermal duties and molal flow rates of interest .....	128
Table 24 ASTM distillation data of products obtained .....	143
Table 25 Costs of energy and sale prices of products used .....	147
Table 26 Summary of hourly operating costs .....	148
Table 27 Summary of hourly product sale values .....	149
Table 28 Summary of yearly economic evaluation .....	150

ศูนย์วิทยทรัพยากร  
จุฬาลงกรณ์มหาวิทยาลัย

## LIST OF FIGURES

	Page	
Figure 1	ASTM distillation apparatus .....	16
Figure 2	Representative ASTM D 86 distillation curves .....	19
Figure 3	Variation of boiling temperature with percent distilled in true-boiling-point distillation of light hydrocarbons .....	19
Figure 4	Comparison of ASTM, TBP, and EFV distillation curves for kerosene .....	20
Figure 5	TBP 50% temperature versus EFV 50% temperature .....	23
Figure 6	TBP temperature difference versus EFV temperature difference .....	23
Figure 7	ASTM 50% temperature versus EFV 50% temperature .....	24
Figure 8	ASTM temperature difference versus EFV temperature difference .....	24
Figure 9	Relationship between ASTM and TBP distillation curves .....	25
Figure 10	Characterization Factor versus boiling point and gravity .....	27
Figure 11	Properties of representative crudes (a) Arabian heavy (b) Arabian light (Berri) .....	29
Figure 12	Crude units .....	33
Figure 13	Breakup of TBP distillation curve into pseudo- components .....	40
Figure 14	Approximate change of specific gravity of inter- mediate-base oils with temperature .....	41

	Page
Figure 15 Molecular weights, critical temperatures, and characterization factors of petroleum fractions .....	43
Figure 16 Molecular weights on true 50% boiling point versus gravities of petroleum fractions .....	44
Figure 17 Winn's Nomograph - Related properties of petroleum fractions .....	45
Figure 18 Molecular weights versus boiling points of petroleum fractions .....	47
Figure 19 Equilibrium Vaporization Constant .....	49
Figure 20 Vapor-liquid equilibria, 40 °F to 800 °F .....	57
Figure 21 ESSO 53-12 Chart - Vapor pressure of hydrocarbons .....	59
Figure 22 Enthalpy of hydrocarbons and petroleum fractions .....	61
Figure 23 Enthalpy of petroleum fractions .....	71
Figure 24 An illustrative theoretical analogue system for mathematical model presentation .....	74
Figure 25 Actual tray numbers in topping column and side-strippers .....	94
Figure 26 Theoretical trays corresponding to system in Fig. 25, obtained by Cecchetti et al. ....	95
Figure 27 Abbreviated display of the component material balance matrix $C_i$ .....	97
Figure 28 Schematic diagram and conditions for the simulation of an existing topping column .....	105
Figure 29 Crude Assay for the Topping Column of Fig. 28 .....	106
Figure 30 The representative crude oil feed was divided into 39 normal boiling point fractions (pseudocomponents) ...	107

	Page
Figure 31 Comparison of simulated stage temperature with plant data .....	119
Figure 32 Comparison of simulated TBP distillation curves with plant data .....	120
Figure 33 Summary of the corresponding product TBP distillation curves .....	129

ศูนย์วิทยทรัพยากร  
จุฬาลงกรณ์มหาวิทยาลัย

## NOMENCLATURES



$A_{ji}$	= Absorption factor
$c$	= Total number of components
$C_i$	= Component material balance matrix
$F$	= Column vector in total material balances, Eq.(29)
$f_i$	= Column vector in component material balances, Eq.(43)
$F_0, F_j$	= Equilibrium function, Eqs.(54,56)
$FS_i$	= Stripping steam flow rate, lb mol/h
$G_j$	= Enthalpy balance function, Eq.(59)
$h_{ji}$	= Component liquid enthalpy, Btu/lb mol
$H_{ji}$	= Component vapor enthalpy, Btu/lb mol
$H$	= $J^{-1}$ , used in Broyden algorithm
$J$	= Jacobian matrix
$K_{ji}$	= Ideal solution K-value
$l_{ji}$	= Component liquid flow rate, lb mol/h
$L_j$	= Total liquid flow rate, lb mol/h
$N$	= Total number of theoretical stages
$NW$	= Sidestream withdrawal plate
$NV$	= Plate below which vapor stream from sidestripper is returned
$NP$	= Pumparound withdrawal plate
$NQ$	= Plate to which liquid-pumparound stream is returned
$NF$	= Feed plate
$NT$	= Bottom plate of main column
$NTOP$	= Top plate of sidestripper
$NBOT$	= Bottom plate of sidestripper

$p_c$	= Partial pressure of water, psia
$p_j$	= Pressure above plate $j$ , psia
$Q_j$	= $j$ -th plate head load, Btu/h
$R_j$	= Mole ratio factor, Eq.(18)
$s$	= Step size
$T_B$	= Average boiling point, R
$T_j$	= $j$ -th plate temperature, C
$T$	= Total material balance matrix
$v_{ji}$	= Component vapor flow rate, lb mol/h
$v_j$	= Total vapor flow rate, lb mol/h
$w_{ji}$	= Component sidestream flow rate, lb mol/h
$w_0, w_j$	= Total sidestream flow rate, lb mol/h
$x$	= Column vector in Newton-Raphson equation, Eq.(66)
$y$	= Vector of functional values, Eq.(75)
$\alpha_j$	= Flow ratio multiplier, Eq.(16)

#### Subscripts

a	= Assumed value
i	= Component number (for water, = c)
j	= Stage number
k	= Calculation trial number