



Cairo University

Predictive Modeling and Optimization of Industrial Penex Isomerization unit

By

Mohanad Magdy Menoufi Mohamed Said

**A Thesis Submitted to the
Faculty of Engineering at Cairo University
In Partial Fulfillment of the
Requirements for the Degree of
MASTER OF SCIENCE
In
Chemical Engineering**

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GIZA, EGYPT

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Title of Thesis:

**Predictive Modeling and Optimization of Industrial Penex
Isomerization unit**

Keywords:

Isomerization, Penex Process, Kinetic Modeling, Predictive Modeling,
Optimization

Summary:

This work presents a model for UOP Hydrogen Once Through (HOT) Penex Process using Aspen HYSYS V7.3. The model relies on routinely taken samples of process streams and normal operating conditions of Penex Unit located in Cairo Oil Refinery. Acquired data sets from the industrial unit have been tested and screened to ensure data validity for building the model and avoiding erroneous results. A reaction network with 20 reactions and 19 components has been used for the reactors model. In addition, rigorous tray by tray simulation of isomerase stabilizer has been utilized to match the performance of plant stabilizer close enough. The model has then been used for studying the effects of process variables on plant performance. Finally, the model has been used in optimizing the operating conditions of the process. Results from optimization scheme showed that considerable savings in isomerase yield and fuel consumption could be accomplished.



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Dedication

For those who are courageous enough to take risks and make sacrifices seeking the best for their families.

Table of Contents

Acknowledgement.....	I
Dedication.....	II
Table of Contents.....	III
List of Tables.....	V
List of Figures	VII
Nomenclature	X
Abstract	XII
Chapter 1: Introduction.....	1
1.1 Gasoline	3
1.2 Gasoline Specifications.....	4
1.2.1 Reid Vapor Pressure and boiling range	4
1.2.2 Octane Number.....	5
1.3 Octane Upgrading Processes.....	6
1.3.1 Naphtha Reforming	7
1.3.2 Alkylation	7
1.3.3 Light Naphtha Isomerization	7
Chapter 2: Literature Review.....	9
2.1 Isomerization Catalysts.....	10
2.1.1 Zeolite Catalysts	11
2.1.2 Chlorinated Alumina Catalysts.....	11
2.1.3 Sulfated Zirconia Catalysts.....	12
2.2 Isomerization Kinetic Modeling	13
2.3 Penex Process	14
2.3.1 Process Description	14
2.3.2 Process Chemistry	17
2.3.3 Process Contaminants.....	19
2.3.4 Process Parameters	20
Chapter 3: Model Development.....	22
3.1 Reactor Model.....	23
3.2 Industrial Data Gathering and Arrangement.....	27
3.3 C ₇₊ De-lumping	27
3.4 Data Screening.....	31
Chapter 4: Model Calibration and Validation.....	35
4.1 Reactor Model Calibration and Parameter Estimation	36

4.1.1 Lead Reactor Calibration	36
4.1.2 Average Activity Parameters	37
4.1.3 Lag Reactor Calibration.....	40
4.1.4 Model Validation	42
4.1.5 Testing Model Prediction Power	45
4.2 Feed Pre-heating	46
4.3 Stabilizer Model.....	49
4.3.1 Tray Efficiency Vs Overall Column Efficiency	49
4.3.2 Column Specifications.....	53
Chapter 5: Process Variables.....	56
5.1 Reactors' Inlet Temperature	57
5.2 Hydrogen/Hydrocarbon mole ratio	60
5.3 Feed rate (LHSV).....	63
5.4 Feed Composition	63
5.4.1 Methyl Cyclo Pentane and Cyclo Hexane	63
5.4.2 Benzene	66
Chapter 6: Process Optimization	69
6.1 Reactors' Temperatures Optimization	70
6.2 Hydrogen: Hydrocarbon mole ratio	71
6.3 Model Application To Process Optimization	71
Chapter 7: Discussion, Conclusions and Recommendations	77
Bibliography	81
Appendix A: Reactors' Models Calibration Results	84
Appendix B: Model Predictions Vs Plant Performance	91
Appendix C: Heat and Material Balance	95
Appendix D: Equipment Specifications.....	103

List of Tables

<u>Table 1-1: Relation between Minimum Ambient Temperature and % Distilled Liquid at 70°C for Acceptable Performance</u>	<u>5</u>
<u>Table 1-2: Relation between Min. Ambient Temp. and 90% Distilled Temp. for Acceptable Performance</u>	<u>5</u>
<u>Table 1-3: Max. Allowable RVP at Ambient Temperature</u>	<u>5</u>
<u>Table 1-4: Variables Effects on Octane Requirements</u>	<u>6</u>
<u>Table 2-1: Typical RON of Isomerate with Different Recycle Schemes (Feed (RON) =69).....</u>	<u>15</u>
<u>Table 2-2:RON Of Normal and Iso-Paraffins.....</u>	<u>18</u>
<u>Table 3-1: Kinetic Parameters Included in Reactor Model</u>	<u>25</u>
<u>Table 3-2: Typical Component Analysis of Feed and Product streams in Penex Unit.....</u>	<u>28</u>
<u>Table 3-3: PNA Composition of C₇₊ Fraction.....</u>	<u>30</u>
<u>Table 3-4: Available and Calculated Properties of C₇₊ Fraction in Feed and Product</u>	<u>31</u>
<u>Table 3-5: Estimated Composition of C₇₊ Fraction in Feed and Product.....</u>	<u>31</u>
<u>Table 3-6: Reactors' Dimensions and Catalyst Properties</u>	<u>32</u>
<u>Table 4-1: Measurements Included in Model Calibration</u>	<u>38</u>
<u>Table 4-2: Applied Weighing Factors</u>	<u>39</u>
<u>Table 4-3: Applied Bounds on Activity Parameters</u>	<u>40</u>
<u>Table 4-4: Estimated Average Activity Parameters for Lead and Lag Reactors</u>	<u>42</u>
<u>Table 4-5: Typical overall efficiency values for some refinery fractionators.....</u>	<u>51</u>
<u>Table 4-6: Components Recovery % in Isomerate Stabilizer</u>	<u>52</u>
<u>Table 4-7: Selected Specifications for Stabilizer Model</u>	<u>54</u>
<u>Table 5-1: Average Composition of Feed Naphtha and Make-Up Gas during Study Period.....</u>	<u>58</u>
<u>Table 5-2: Operating Scheme for Lead and Lag Reactors.....</u>	<u>60</u>
<u>Table 6-1: Operating Conditions of the Unit at the Base Operating Point and Limit Bounds Induced by Process Licensor</u>	<u>72</u>
<u>Table 6-2: Process Performance at Base and Optimum Operating Point</u>	<u>75</u>

Table 6-3: Net Heating Value of Make-up Gas	76
Table A.1:Model Calibration Results	85
Table B.1:Model Predictions Vs Plant Performance	92
Table C.1:Process Streams Conditions	96

List of Figures

Figure 1-1: Distribution of Refinery Capacities	2
Figure 1-2: Typical Block Flow Diagram of a Coking Refinery	3
Figure 2-1: Effect of Temperature on Isomers Yield.....	10
Figure 2-2: Comparison of the Activity of Different Isomerization Catalysts	11
Figure 2-3: Process Flow Diagram of Zeolite Catalyst Based Isomerization	12
Figure 2-4: Process Flow Diagram of Chlorinated Alumina Based Isomerization	12
Figure 2-5: Process Flow diagram of Sulfated Zirconia Based Isomerization	13
Figure 2-6: UOP Hydrogen Once Through Penex Process	14
Figure 2-7: Penex Process with Deishexanizer.....	16
Figure 2-8:Penex/Molex Process with Recycle of Normal Paraffins	16
Figure 2-9: Penex Process with Normal Paraffins and Methyl Pentanes Recycle.....	16
Figure 3-1: HYSYS Isomerization Model Reaction Network.....	24
Figure 3-2: Overall Modeling Strategy.....	26
Figure 3-3:Variation of C7+ Feed Content.....	27
Figure 3-4: Mass Balance Error For Acquired Data Sets	33
Figure 3-5: Hydrogen Balance Error For Acquired Data Sets.....	33
Figure 4-1: Estimated Activity Parameters For Lead Reactor (A) Global Activity;(B)Isomerization Activity;(C) Hydrocracking Activity;(D) Hydrogenation Activity;(E) Ring Opening Activity;(F) Heavy Activity	41
Figure 4-2:Estimated Activity Parameters for Lag Reactor (A) Global Activity;(B)Isomerization Activity;(C)Hydrocracking;(D)Hydrogenation Activity;(F)Ring Opening ;(F)Heavy activity ..	43
Figure 4-3: Plant versus Model yields with data sets used for lead reactor calibration.....	44
Figure 4-4: Plant versus Model yields with data sets used for lag reactor calibration	44
Figure 4-5: Plant versus Model yields for 4 months after calibration (Lead Reactor)	45
Figure 4-6: Plant versus Model yields for 4 months after calibration (Lag reactor)	46
Figure 4-7: PROII Pre-Heat Train Flow Sheet	48

Figure 4-8: Stabilizer Temperature Profile	54
Figure 4-9: Penex Isomerization Unit Model	55
Figure 5-1:A- Effect of Lead Reactor Inlet Temperature on RON; B- Variation of (I-C5/C5)% with Lead Reactor Inlet Temperature; C- Variation of (2,2DMB/C6)% with Lead Reactor Inlet Temperature; D- Variation of (2,3DMB/C6)% with Lead Reactor Inlet Temperature; E- Effect of Lead Reactor Inlet Temperature on Hydrogen Consumption in Lead Reactor; F- Effect of Lead Reactor Inlet Temperature on Isomerase Yield. Lag Reactor Inlet Temperature = 120 °C, H ₂ : HC = 0.1565, A6 = 2.99 wt. %, LHSV = 1.15 hr ⁻¹	59
Figure 5-2: A- Effect of Lag Reactor Inlet Temperature on RON; B- Variation of (I-C5/C5)% with Lag Reactor Inlet Temperature; C- Variation of (2,2DMB/C6)% with Lag Reactor Inlet Temperature; D- Variation of (2,3DMB/C6)% with Lag Reactor Inlet Temperature; E- Effect of Lead Reactor Inlet Temperature on Hydrogen Consumption in Lag Reactor; F- Effect of Lag Reactor Inlet Temperature on Isomerase Yield. Lead Reactor Inlet Temperature = 124 °C, H ₂ :HC = 0.1565, A6 = 2.99 wt%, LHSV = 1.15 hr ⁻¹	61
Figure 5-3:A- Effect of H ₂ :HC Ratio on Isomerase Yield; B- Effect of H ₂ :HC Ratio on RON of Isomerase; C- Effect of H ₂ :HC Ratio on PIN. Lead Reactor Inlet Temperature = 124°C, Lag Reactor Inlet Temperature = 120 °C, A6 = 2.99 wt%, LHSV = 1.15 hr ⁻¹	62
Figure 5-4:A- Effect of Feed Rate (LHSV) on PIN; B- Effect of Feed Rate (LHSV) on Isomerase Yield. Lag Reactor Inlet Temperature = 120 °C, H ₂ :HC = 0.1565, A6=2.99wt%	63
Figure 5-5:A- Effect of Feed MCP Content on PIN; B- Effect of Feed CH Content on PIN; C- Effect of Feed MCP Content on RON; D- Effect of Feed CH Content on RON; E- Effect of Feed MCP Content on Isomerase Yield; F- Effect of Feed CH Content on Isomerase Yield; G- Effect of Feed MCP Content on Total Hydrogen Consumption; H- Effect of Feed CH Content on Total Hydrogen Consumption; I- Effect of Feed MCP Content on Hydrogen Consumption in Lag Reactor; J- Effect of Feed CH Content on Hydrogen Consumption in Lag Reactor. Lead Reactor Inlet Temperature = 124 °C, Lag Reactor Inlet Temperature = 120°C, LHSV = 1.15hr ⁻¹	64
Figure 5-6:A- Variation of Feed Benzene Content; B- Effect of Feed Benzene Content on Lead Reactor Temperature Rise; C- Effect of Feed Benzene Content on Isomerase RON; D- Effect of Feed Benzene Content on PIN in Lead Reactor; E- Effect of Feed Benzene Content on Isomerase Yield; F- Effect of Feed Benzene Content on Hydrogen Consumption in Lead Reactor. Lead Reactor Inlet Temperature = 124 °C, Lag Reactor Inlet Temperature = 120°C, LHSV = 1.15 hr ⁻¹	68
Figure 6-1: Equilibrium i-C5/C5 Ratios in Vapor and Liquid Phases	71

<u>Figure 6-2: Variation of Isomerase Yield with Reactors Inlet Temperatures</u>	<u>73</u>
<u>Figure 6-3: Variation of Paraffin Isomerization No.with Reactors Inlet Temperatures</u>	<u>73</u>
<u>Figure 6-4: Variation of Isomerase RON with Reactors Inlet Temperatures.....</u>	<u>74</u>

Nomenclature

A = Exchanger Heat Transfer Area
ASTM=American Society For Testing And Materials
A6 = Benzene
C1 = Methane
C2 = Ethane
C3 = Propane
i-C4 = Isobutane
n-C4 = Normal Butane
i-C5 = Isopentane
n-C5 = Normal Pentane
n-C6 = Normal Hexane
n-C7 = Normal Heptane
CH = Cyclo Hexane
2,2-DMB = 2,2-dimethylbutane
2,3-DMB = 2,3-dimethylbutane
E = Overall Column Efficiency
ETBE = Ethyl Tertiary Butyl Ether
FCC = Fluid Catalytic Cracking
 F_T = LMTD Correction Factor
H factor_i = Weight fraction of Hydrogen in component i
I = Parameter for Calculating Refractive Index at 20°C
Isomerate = Liquid Product of Isomerization Process
LHSV = Liquid Hourly Space Velocity
LHV = Low Heating Value
m = Parameter Calculated From Refractive Index and Molecular Weight
MBP7 = Multi Branched Heptanes
MCH = Methyl Cyclohexane
MCP = Methyl Cyclopentane
MON = Motor Octane No.
2MP = 2-Methyl Pentane
3MP = 3-Methyl Pentane
 M_w = Molecular Weight
MTBE = Methyl Tertiary Butyl Ether
n = Refractive Index at 20°C
5N5 = Cyclopentane
5N7 = Five Ring, Seven Carbon Naphthene
6N7 = Six Ring, Seven Carbon Naphthene
NP7 = Normal Heptane
PIN = Paraffin Isomerization Number = $i\text{-C}_5/\text{C}_5 + 2,2\text{-DMB}/\text{C}_6 + 2,3\text{-DMB}/\text{C}_6$
PON = Posted Octane No.
PSA = Pressure Swing Adsorption
Q = Duty
Reformat = Catalytic Naphtha Reforming Liquid Product
RON = Research Octane No.
RVP = Reid Vapor Pressure
SBP7 = single branched heptanes

SG = Specific Gravity
 TAME = Tertiary Amyl Methyl Ether
 ΔT_{model} = Temperature Rise in Reactor Model
 ΔT_{plant} = Temperature Rise in Plant Reactor
 ΔT_{LM} = Log Mean Temperature Difference (LMTD)
 U = Overall Heat Transfer Coefficient
 VDU = Vacuum Distillation Unit
 w_i = Weighing Factor for Component i
 X_i = Mole, Volume or Mass Fraction of Component i
 $X_{\text{model}-i}$ = Mass Fraction of Component i in Model Outlet Stream
 $X_{\text{plant}-i}$ = Mass Fraction of Component i in Plant Reactor Outlet Stream
 x_n = Naphthenes Volume %
 x_p = Paraffins Volume %
 y_n = Actual Concentration of Vapor Leaving Plate n
 y_n^* = Concentration of Vapor in Equilibrium with Liquid Leaving Plate n
 y_{n+1} = Actual Concentration of Vapor Entering Plate n
 ψ = property of a petroleum fraction
 ψ_i = property of a pure component i
 θ = known property of C7+ fraction
 η_M = Murphree Efficiency
 μ = Viscosity
 α = Relative Volatility