

**OPTIMIZATION OF KADUNA REFINERY AND
PETROCHEMICAL COMPANY (KRPC) CRUDE
DISTILLATION UNIT I (CDU I)
USING HYSYS**

**A THESIS PRESENTED TO
CHEMICAL ENGINEERING DEPARTMENT
FEDERAL UNIVERSITY OF TECHNOLOGY
MINNA-NIGER STATE NIGERIA**

BY

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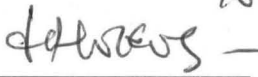
**IN PARTIAL FULFILMENT OF THE
REQUIREMENT FOR THE AWARD OF M.ENG
DEGREE IN CHEMICAL ENGINEERING.**

MARCH, 2008.


CERTIFICATION

This thesis titled **OPTIMIZATION OF KADUNA REFINERY AND PETROCHEMICAL COMPANY (KRPC) CRUDE DISTILLATION UNIT I (CDU I) USING HYSYS** by **MOHAMMED JIBRIL (M.ENG/SEET/2005/1371)** meets the regulations governing the award of the degree of M.Eng of the Federal University of Technology, Minna and is approved for its contribution to scientific knowledge and literary presentation.

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DEDICATION

This work is dedicated to **ALMIGHTY ALLAH (SWT)**.

DECLARATION

I, **MOHAMMED JIBRIL**, declare that this project is a result of my personal research work and has not been presented elsewhere for the award of any certificate.

Information derived from published and unpublished works have been duly acknowledged.



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ACKNOWLEDGEMENTS

First of all, I would like to thank Allah for giving me the strength and perseverance to complete this project and my late Father for giving me a good legacy may his soul find a peaceful abode Amin.

I would then like to express my profound gratitude to my loving Mother Mrs Adama Jumai and my siblings Isiak, Fatima, Fausiyah, Abdullah and Abdulrasaq for their love, care and support during the course of the program. I am very grateful indeed.

I also want to thank Mr and Mrs Kazeem Olayinka Muraina and Mr Fred Amao Jonathan for their financial and moral support, not forgetting my cronies Engr. Abdulmajeed Jimoh, Nurudeen Abdulazeez, Sunmonu Said, Niyirash, Late Dr Suleiman (SDS), Jamiu Aliyu, Nurudeen Alowonle, TJ, John, Solex and Sani for their immense support.

To all my colleagues Engr. Mohammed Jibril Isah, Mrs Anyakora, Mrs Adeola and most especially Mallam Hassan Funsho Akande for his assistance and contribution towards the success of this thesis, I wish to say thank you for all the hectic and memorable times we shared.

Special regard to my Supervisor Dr D.F Aloko for his patience, constructive criticism and painstaking effort. I wish to also thank Prof. K.R Onifade for his Fatherly role and the entire staff of the department, especially Prof. J.O Odigure and the Head of Department Dr M.O Edoga for the support and words of encouragement. Finally, I would like to thank the entire staff of Kaduna Refinery and Petrochemicals Crude Distillation Unit for their contribution and useful information and all those that contributed in one way or another in completing this project but too numerous to mention.

ABSTRACT

The optimization of chemical processes has attracted attention because, in the face of growing competition, it is a natural choice for reducing production costs, improving product quality, meeting safety requirements or environmental regulations. Optimization of crude distillation column of Kaduna Refinery and Petrochemical Company by computer simulation (HYSYS) has been carried out. The optimization technique used is Sequential Quadratic Programming (SQP) optimization technique. The column was operated with better performance while keeping the product quality constraints within the specified limits.

The optimization objective function is Naphtha product volume flow rate. The optimization carried out shows that the plant has a profit analysis of ₦24,457,543.43, while the base case has a profit analysis of ₦22,375,349.71. The constraint variables used for the optimization are the Condenser and Trim duty. The optimization also shows that Naphtha product volume flow rate is 228.6m³/h while that of the base case is 200.3m³/h respectively; hence the optimum value of the Naphtha product volume flowrate is 228.6m³/h.

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NOMENCLATURE

Symbol	Name	Unit
Min	Minimum	
S	Range Property	
X	Internal Variables	
V	External (model) Variables	
δ	Optimizer Perturbation property	
V_j	Perturbing Variable	
C_j	Constraints Variables	
CPU	Central Processing Unit	
Unit Op	Unit Operations	
Jac Offset	Jacobian Offset	
Jac Num	Jacobian Number	
E	Exponential	
BPSD	Barrels Per Stream Day	
CDU	Crude Distillation Unit	
UQCC	Ughelli Quality Control Centre	
KRPC	Kaduna Refinery and Petrochemical Company	
AGO	Atmospheric Gas Oil	
KeroSS	Kerosene Side Stripper	
AGOSS	Atmospheric Gas Oil Side Stripper	
SFS	Sub Flow Sheet	
SMO	Simultaneous Modular Optimization	

DRU	Data Reconciliation Utility Stream
Optim	Optimization
SS_LP	Single-Shot Linear Programming
SLP	Sequential Linear Programming
SQP	Sequential Quadratic Programming
# Stages	Number of Stages
Ovhd	Overhead
Atm	Atmospheric
PFD	Process Flow Diagram
\$	Dollar
Z Factor	Compressibility Factor
DRU	Data Reconciliation Utility

CHAPTER ONE

1.0 INTRODUCTION

The Kaduna Refinery and Petrochemical Company (KRPC) was commissioned in 1980, with an initial capacity of 100,000 Barrels Per Stream Day (BPSD). It has a Fuel Plant Crude Distillation Unit I (CDU I) and a Lube Plant Crude Distillation Unit II (CDU II). The Fuel Plant was designed to process 50,000 Barrels Per Stream Day (BPSD) but was later upgraded to 60,000 Barrels Per Stream Day (BPSD). It processes Escravos light crude oil and Ughelli Quality Control Centre (UQCC) crude oil while the Lube Plant has capacity to process 50,000 Barrels Per Stream Day (BPSD) of imported Paraffin rich crude oil for the manufacture of lubricating oils. The crude oils available in Nigeria can not produce the whole range of fractions for the production of lubricating oils, hence Nigerian National Petroleum Corporation (NNPC) imports from Venezuela, Kuwait or Saudi Arabia.

Crude distillation units (CDU) of Kaduna Refinery and Petrochemical Company (KRPC) are the most strategic units for the processing of the crude oil. The process in the units involves passing the crude oil through preheat trains of exchangers prior to the main distillation or fractionation and the products are also cooled before sending to storage units. Atmospheric Crude Columns are one of the most important pieces of equipment in the petroleum refining industry. Typically located after the Desalter and the Crude Furnace, the Atmospheric Tower serves to distil the crude oil into several different cuts. These include naphtha, kerosene, light diesel, heavy diesel and Atmospheric Gas Oil (AGO) (Chiyoda, 1980).

1.1 Background

The optimization of chemical processes has attracted attention because, in the face of growing competition, it is a natural choice for reducing production costs, improving product quality, meeting safety requirements or environmental regulations. From an industrial perspective, the main objective is often economic and is stated in terms such as return, profitability or payback time of an investment (Smith, 2005).

The potential gains of optimization could be significant. However there have been only a few attempts to optimize operations through computer simulation. The optimization of Kaduna Refinery and Petrochemicals will bring financial gains to the company and the country.

The recipes developed in the laboratory are implemented conservatively in production, and the operator uses heuristics gained from experience to adjust the process periodically, which might lead to slight improvements from batch to batch (www.aspentech.com.paper). In the past, the stumbling blocks for the use of computer simulation in industrial practice have been:

- *Reliable Modeling Tools*
- *Reliable Measurements*

Nevertheless, there is a clear indication that recent advances in both computer simulation software and sensor technology are helping to remove the two handicaps mentioned above and, thus, are opening up new avenues to reliable process optimization. Software tools such as Hysys, SimuSolv, SPEEDUP, ASPEN Plus, or gPROMS (Himmeblau et-al, 2005), have helped reduce the time and effort necessary to obtain reliable models.

1.2 Aim and Objectives

The aim of this research work is to carry out optimization of crude distillation column of Kaduna Refinery and Petrochemical Company by computer simulation using HYSYS.

This aim can be actualized through the realization of the following objectives:

1. To obtain the maximum production capacity of the products: Naphtha, Kerosene, Diesel and Atmospheric Gas Oil.
2. To obtain the minimum production capacity of Atmospheric Residue
3. To obtain Minimum Production Cost and
4. To obtain Optimum Venture Profit

1.3 Scope of the Project

The Scope of this Project encompasses the simulation of the KRPC Crude Distillation Unit (Base Case) and subsequently carrying out the Optimization on the Crude Distillation Unit (Optimized Case) and determining the resulting profit using Hysys Simulation Software Package called the Sequential Quadratic Programming (SQP) Optimizer.

1.4 Approach

The research would consist of the following approach:

1. **Collection of Data:** Design data, Operating Data and Piping and Instrumentation Diagram of Crude Distillation Unit (CDU) of Kaduna Refinery and Petrochemical Company (KRPC) would be collected from KRPC.

2. Constructing a Crude Distillation Column Model in a Process Simulator:

Building the crude distillation column and the side operating equipment of crude distillation column model of KRPC in HYSYS using the data collected in 1 above.

3. Computer Simulation: Computer simulation of the model constructed in 2 would be carried out using HYSYS.

4. Optimization: Optimization of crude distillation column is carried out using HYSYS Derivative Utility to:

- Define Process Constraints and Variables.
- Define the Objective Function
- Run the Optimizer.

5. Results: Results are obtained from the computer simulation and optimization carried out in step 3 and 4 above and the following parameters are estimated:

1. Maximum capacity of Naphtha produced from the CDU column
2. Maximum capacity of Kerosene produced from the CDU column
3. Maximum capacity of Diesel produced from the CDU column
4. Maximum capacity of Atmospheric Gas Oil produced from the column
5. Minimum Cost of Production
6. Optimum profit obtained from the process.

CHAPTER TWO

2.0 LITERATURE SURVEY

The literature review of this work will be looked at under the following titles.

2.1 Crude Distillation Unit of the Kaduna Refinery and Petrochemical Company

This unit is a crude oil processing facility consisting of a pre-fractionation train used to heat the crude liquids, and an atmospheric crude column to fractionate the crude into its straight run products. Preheated crude (from a preheat train) is fed to the pre-flash drum, where vapours are separated from the crude liquids. The liquids are then heated to 650°F in the crude furnace. The pre-flash vapours bypass the furnace and are re-combined, using a mixer, with the hot crude stream. The combined stream is then fed to the atmospheric crude column for separation. The crude column is a refluxed absorber, equipped with three pump-around and three side stripper operations (Chiyoda, 1980).

The main column consists of 29 trays plus a partial condenser. The tower feed enters on stage 28, while superheated steam is fed to the bottom stage. In addition, the trim duty is represented by an energy stream feeding onto stage 28. The Naptha product, as well as the water stream Waste water, is produced from the three-phase condenser. Crude atmospheric Residue is yielded from the bottom of the tower. Each of the three-stage side strippers yields a straight run product. Kerosene is produced from the reboiled Kerosene side stripper, while Diesel and AGO (Atmospheric Gas Oil) are produced from the steam-stripped Diesel and AGO side strippers, respectively (Chiyoda, 1980).

2.1.1 Crude distillation unit of KRPC

The target capacity of CDU-1 after debottlenecking is 60,000 BSPD (1 B=159 litres) of Gulf Escravos crude oil. Crude is formed by a series of hydrocarbon with different characteristics. To use, it must be divided into groups such that each group has well defined characteristics. Distillation takes advantage of one of the physical characteristics, that is, boiling point. The basic mechanics therefore is heating the crude (without changing the structure of any components) and then fractionating it into groups. The characteristics of these groups are linked to the market's need for commercial products and to the specifications of the process plants for the products destined to undergo subsequent treatment.

Tables 2.1 through 2.5 are the crude assay data of KRPC Crude Distillation Unit.

Table 2.1: Bulk Crude Properties (KRPC, 2007)

Bulk Crude Properties	
MW	300.00
API Gravity	48.75

Table 2.2: Light Ends Liquid Volume (KRPC, 2007)

Light Ends Liquid Volume Percent	
i-Butane	0.19
n-Butane	0.11
i-Pentane	0.37
n-Pentane	0.46

Table 2.3: TBP Distillation (KRPC, 2007)

TBP Distillation Assay		
Liquid Volume Percent Distilled	Temperature (°F)	Molecular Weight
0.0	80.0	68.0
10.0	255.0	119.0
20.0	349.0	150.0
30.0	430.0	182.0
40.0	527.0	225.0
50.0	635.0	282.0
60.0	751.0	350.0
70.0	915.0	456.0
80.0	1095.0	585.0
90.0	1277.0	713.0
98.0	1410.0	838.0

Table 2.4: API Gravity Assay (KRPC, 2007)

API Gravity Assay	
Liq Vol% Distilled	API Gravity
13.0	63.28
33.0	54.86
57.0	45.91
74.0	38.21
91.0	26.01

Table 2.5: Viscosity Assay (KRPC, 2007)

Viscosity Assay		
Liquid Volume Percent Distilled	Viscosity (cP) 100°F	Viscosity (cP) 210°F
10.0	0.20	0.10
30.0	0.75	0.30
50.0	4.20	0.80
70.0	39.00	7.50
90.0	600.00	122.30

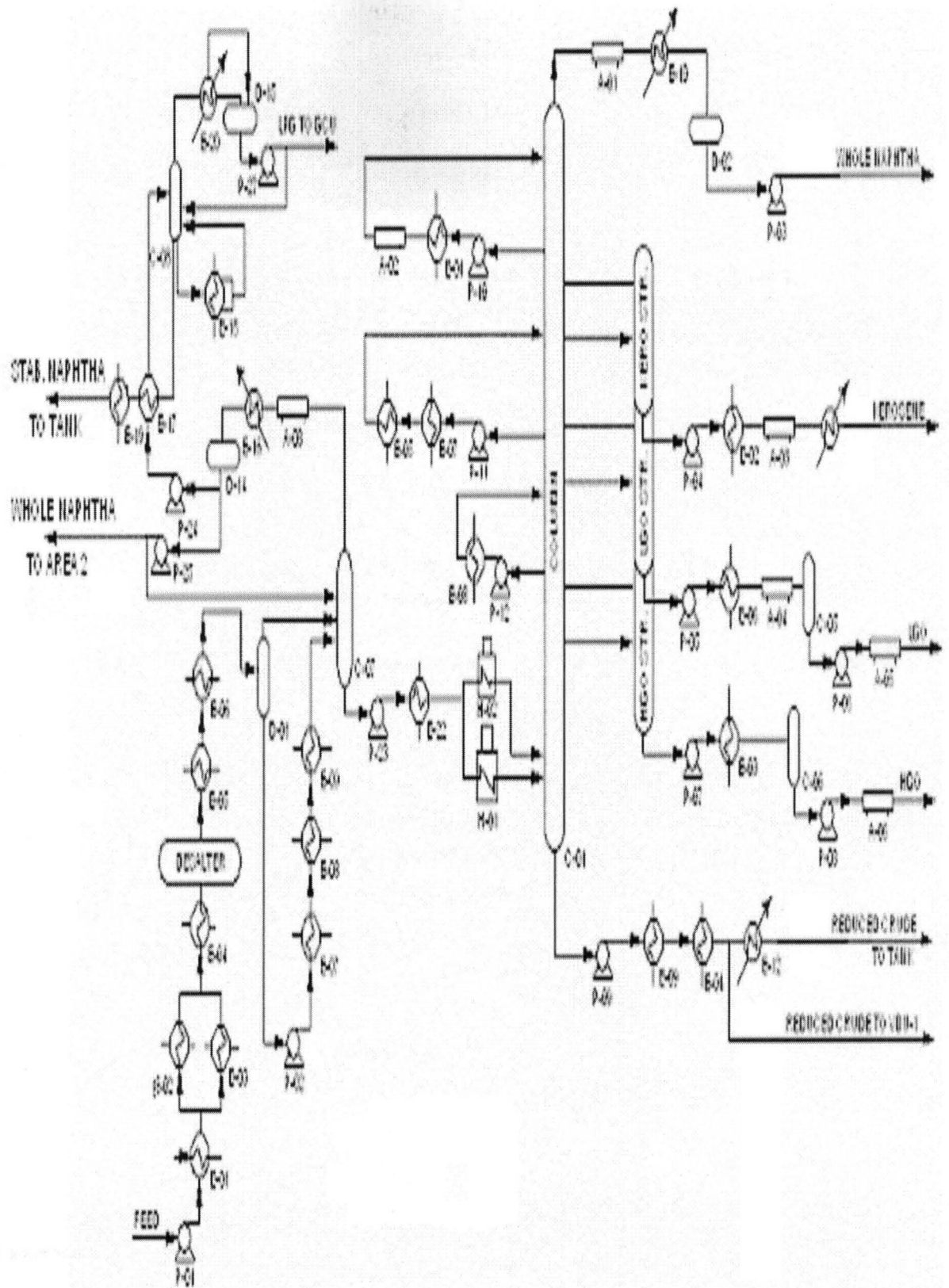


Figure 2.1: CDU-1 Schematic Diagram

2.2 Optimization in Process Simulator

Optimization within HYSYS is based on a simultaneous modular approach. A flow sheet model is developed as a collection of Sub-flow sheets (SFS or the modular blocks) are connected through streams. Within each Sub-flow sheets are a collection of unit operations and streams that are appropriate to be solved together. During the course of the optimization run, each Sub-flow sheet is solved using one of the standard HYSYS solvers (non-sequential modular or one of the available column solvers). When the model is being posed to the optimizer, each product stream from one Sub-flow sheet that serves as a feed stream to the main Sub-flow sheet is "torn" (www.aspentech.com.paper).

The act of tearing the stream creates a collection of connection equations which the optimizer solves as part of its calculations. In the case of nested Sub-flow sheets, the tearing occurs at the terminal locations (i.e., between the stream which is calculated as the product of one unit operation, and the stream which feeds the next unit operation). There are no intermediate tears constructed. Recycle locations in the flow sheet should be defined at the transition across a Sub-flow sheet boundary. This additional transfer basis allows the flow sheet to be initialized correctly, and then have the recycle replaced by connection equations when the model is posed to the optimizer. Within each of the Sub-flow sheets are a number of decision variables, true process constraints and objective function variables. These are individually selected and configured by the user and are automatically associated with the corresponding block when the problem is posed to the optimizer.

Upon configuration of the flow sheet, Derivative Utilities can be attached to the various Sub-flow sheet operations. These utilities allow the tearing of the appropriate streams to be invoked, and the various optimization objects (decision

variables, constraints, objective function variables) collected into lists which are then provided to the optimizer. When the optimizer is invoked, it accesses these lists from each of the utilities to construct its solution matrix. During the course of its solution, the optimizer configures the necessary information from each of the objects to determine aspects such as step size, derivative evaluations etc. In the simultaneous modular approach, the blocks are treated as a matrix of variables (decision and tear) and constraints (true process constraints and connection equations) (www.aspentech.com.paper).

The derivatives that the optimizer then sees from any block are of the entire constraints vector with respect to each individual variable within the block. If the block contains variables which are part of the objective function, the gradient is also determined for each of the variables. During the optimization, values are returned to the flow sheet through the utilities to be evaluated by the models, with the calculated results (tear equation residuals, process constraint values, objective function, etc.) returned to the optimizer. The interaction between the optimizer and the flow sheet continues until the defined solution criteria are met (www.aspentech.com.paper).

2.2.1 Role of the sub-flow sheet

In the standard HYSYS modeling environment, the sub-flow sheet lets you provide a logical grouping of operations to facilitate understanding of the process behavior. In addition, it provides the mechanism to encapsulate a solver (i.e., the Column sub-flowsheet) or to use different fluid packages (thermodynamics, component slates, etc.) within a simulation. For optimization, the sub-flowsheet provides the same benefits plus a number of additional capabilities for the simultaneous modular approach. Foremost, it provides a location where the standard propagation of information can be broken. Once a model is torn for optimization,

information does not propagate from one sub-flowsheet to another. This limits calculations to only those needed at a point in time. Similarly, by selecting the structure of the Sub-flowsheets appropriately, unnecessary equations are never posed to the optimizer.

In addition, if derivatives are being generated numerically, the potential for noise in the generated derivatives is minimized by constructing suitably sized Sub-flowsheets.

For operations that deliver analytical derivatives, these must be encapsulated within a single sub-flowsheet. For example, HYSYS columns being solved by the Newton solver are able to deliver the Jacobian matrix to the optimizer directly. Extension unit operations that deliver analytical derivatives are handled in the same manner (www.aspentech.com.paper).

2.2.2 Simultaneous modular optimization

Simultaneous Modular Optimization (SMO) is a hybrid between Sequential Modular and Open Equation forms of optimization. It uses modular solvers to solve the unit operations themselves, and the Optimizer solver to solve both the Optimization and connection equation problems.

2.2.3 Implementation in HYSYS.RTO

In HYSYS.RTO, the SMO is facilitated by the development of Optimization Objects (which provide a generic interface to flowsheet variables), configuration utilities (Data Reconciliation and Derivative) and flowsheet tearing. The act of tearing the flowsheet blocks the propagation of information across the torn location, creating a set of connections equations which are exposed to the Optimizer for solution as part of the optimization problem.

2.2.3.1 Overview

For the HYSYS user, the key pieces to configuring an optimization or data reconciliation problem are:

- Optimization Objects. A generic set of objects used to identify the underlying flowsheet variable and provide the necessary configuration information for use by Optim or Estim.
- Collection Utilities. Utilities used to identify the “pieces” of the flowsheet which are to be exposed to Optim or Estim.
- Optim and Estim parameters. Tolerances and flags. The mechanics for creating either a Data Reconciliation or Optimization problem are essentially identical.

The only differences are as follows:

- Optimization object types being used
- Optim or Estim properties
- Tolerances and flags being configured
- Specific procedures to the type of problem being solved

2.2.3.2 Optimization objects

Optimization objects are the mechanism of identifying the flowsheet variables which are to be considered as part of the problem. The optimization and data reconciliation routines have the ability to set and retrieve flowsheet values as well as the necessary configuration parameters through the optimization object. While there are a number of different optimization object types, they all serve the same basic function. The primary differences between the optimization objects are the properties they contain, and how Optim or Estim treats them. For flowsheet optimization, there are:

- *Optimization Variable*. Decision variables for the optimization that must be specified (blue) variables.
- *Constraints*. True process constraints, bounded variables that are initiated by the user. These must be calculated (black) variables.
- *Objective Function Variables*. A variable that is part of the overall objective function. Each variable has its own defining equation, the results of which are combined into a single flowsheet objective function. These must be calculated (black) variables.

For Data Reconciliation and Parameter Estimation, there are:

- *Digital Control System (DCS) Tags*. Variables for which you have a set of measurements, which are used to calculate offsets in the measurements and update fitting parameters. These can be either specified or calculated variables.
- *Fitting Parameters*. Variables whose value is to be directly adjusted to match the supplied data. These must be specified (blue) variables. There is a third type of Optimization Object used for Data Reconciliation called a DRU Stream (Data Reconciliation Utility Stream). This is essentially a data holder, i.e., it allows for multiple sets of stream data, each corresponding to a different data set, to be supplied by you. These values are taken as supplied; no offsetting is calculated for these streams (www.aspentech.com.paper).

2.2.3.3 Collection utilities

The derivative and data reconciliation utilities are shown under collection utilities of Hysys.

2.2.3.4 Derivative and data reconciliation utility

There are two utilities used by HYSYS.RTO to provide the primary interface between the flowsheet model and the solver:

- Data Reconciliation Utility and Derivative Utility.

Their primary purpose is to collect appropriate optimization objects which are then exposed to the solvers. These utilities are first "attached" with unit operation(s) within the flowsheet model. Then, based on the types of optimization objects that the derivative utility is using for optimization, it collects those objects of the correct types which are attached to variables that are related to the targeted unit operations and their corresponding streams. It is the corresponding lists of "variables" and "constraints" that are exposed to Optimization.

2.4 Optimizer Interface

The Optimizer interface in HYSYS provides the collection points for the utilities within the flowsheet. Depending on the mode, the Optimizer invokes either Estim (Data Reconciliation and Parameter Fitting) or Optim (Optimization) and provides the necessary interfaces back into the process model.

2.5 Data Reconciliation/Parameter Estimation Problem

2.5.1 General procedure

1. Build the flowsheet.
2. Install a Data Reconciliation utility.
3. Select the unit operations from the flowsheet that are associated with the variables to be fit, or for which you have measured the data. The streams that are attached to the unit operations are automatically obtained at the same time.
4. Install Fitting Parameters from the Utility and attach them to the appropriate flowsheet variables to be fit.
5. Supply appropriate values for the Fitting Parameters.
6. Install Digital Control System (DCS) Tags and attach them to flowsheet variables for which you have measured data.

7. Supply required values for the Tags.
8. Supply the measured data.
9. If necessary, turn on the multiple data set option for attached streams, and supply corresponding data.
10. Set the appropriate Estim properties and tolerances and flags.
11. Invoke the HYSYS Optimizer F5 and turn on Data Reconciliation mode.
12. Identify the utility containing the unit operations and streams being reconciled.
13. Start the data reconciliation.

2.6 Optimization Problem

2.6.1 General procedure

1. Build the flowsheet.
2. Install a Derivative utility.
3. Select Flowsheet Wide for the Unit Operation.
4. Install Optimization Variables from the utility and attach them to the appropriate flowsheet variables.
5. Supply appropriate values for the Optimization Variables.
6. Install Constraints and attach them to appropriate flowsheet variables.
7. Supply required values for the Constraints.
8. Install the objective function object(s) and attach them to appropriate flowsheet variables.
9. Configure the appropriate prices for the objective function objects.
10. Invoke the Optimizer F5 and select Optimization.
11. Change appropriate Optim properties and tolerances and flags.
12. Start the Optimization.

2.6.2 Optimization objects

The Optimization object types which are used for optimization problems is shown in Table 2.6

Table 2.6: The Optimization Object Type Window

Type	Description
Optimization Variable	Decision variables for the optimization that must be specified (blue) variables.
Constraints	True process constraints, bounded variables and are instantiated by the user. These must be calculated (black) variables.
Objective Function Variables	A variable which is part of the overall objective function. Each variable has its own defining equation, the results of which are combined into a single flowsheet objective function. These must be calculated (black) variables.

2.7 Optimization Object Installation

Optimization objects appropriate for the utility (in the case of the Derivative utility - Optimization Variables, Constraints and Objective Function variables) can be added directly from the view. Use the drop-down list in the upper right corner of the Derivative Utility Configuration group, to select one of the three options. By selecting the appropriate option and clicking the Add button, the corresponding selection view is displayed (www.aspentech.com.paper):

the Objective Function object. The default formula for an Objective Function object is variable value X price.

The calculations performed for determining the individual contribution of that object to the overall objective function are done in display units. For example, if the objective function object is attached to a Liquid Volume Flow variable, and the current display units are in Barrels/Day, then the actual display value (1000 bbl/day) is used in determining the contribution to the objective function. You can create a new unit set (Tools/Preferences) for this purpose.

2.7.2 Derivative analysis

The Derivative Analysis tab of the utility property view provides access to the Jacobian and Gradient calculation mechanism used during the solution. Examine different perturbation sizes and single and two sided gradient calculations to see their impact on the calculated Jacobian and gradient for the variables.

Filtering is provided to allow examination of subsets of the overall variable and constraint lists. In addition, examine the model noise to determine if tighter solution tolerances on the individual unit operations (i.e., Columns) are necessary. Typically, a tighter solution tolerance requires more individual calculations at any phase, but improves the quality of the Jacobian being returned to Optim and reduces the time of the overall problem solution (www.aspentech.com.paper).

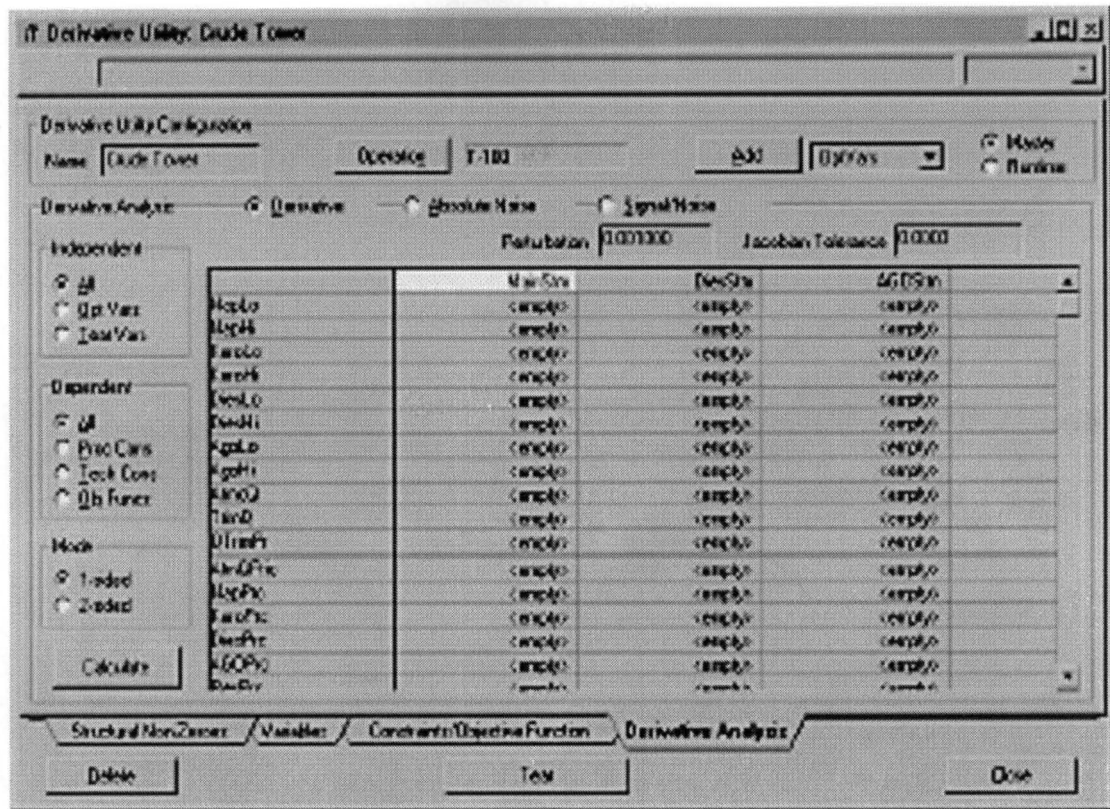


Fig 2.3: Derivative Utility Window

When the calculations are complete, examine the individual Jacobian elements, or the Gradient, as well as the noise of the model. While the default solution tolerances for unit operations is valid for modelling purposes, experience shows that a tighter tolerance is more appropriate for Jacobian evaluations (where small changes are being applied to determine the direction).

This is the original absolute model noise (comparison of the original value of the constraint, to the calculated value when the variable is returned to its starting value), while the screen below shows the values when a tighter tolerance is used in the calculations (www.aspentech.com.paper).

	MaxMin	DistMin	ADCSra	GradProd
WgtLo	0.00000797	0.00000002	0.00000001	0.00000002
WgtHi	0.00001934	0.00000002	0.00000001	0.00000002
WgtLo	0.00000718	0.00000002	0.00000001	0.00000002
WgtHi	0.00000728	0.00000002	0.00000001	0.00000002
DistLo	0.00000445	0.00000001	0.00000000	0.00000001
DistHi	0.00000701	0.00000001	0.00000000	0.00000001
WgtLo	0.00000352	0.00000001	0.00000000	0.00000001
WgtHi	0.00000230	0.00000001	0.00000000	0.00000001
DistLo	0.2294617	0.00004001	0.00001582	0.00005429
Time	0.00250171	0.00001114	0.00000254	0.00001476

Figure 2.4: Tolerance Dialog Box

In addition to examining the affects of the perturbation size, gradient types, etc., on the calculated Jacobian and Gradient, you can also use the Derivative Analysis tab to determine the size of the Ranges best suited for the optimization problem. The size of the perturbation which applied to the variable is determined by the Range perturbation. The Range is different from the span (which is used by the Optimizer in the Jacobian normalization, and is calculated as the Maximum to the Minimum).

	MinSpan	MaxSpan	ADCSpan	GenProd
Wght	0.00013478	-0.00011657	0.00001680	-0.00011528
Wght	0.00027036	-0.00035147	0.00000600	-0.00017703
Wght	0.00014193	0.00001724	0.00006875	-0.00005210
Wght	0.00016334	-0.00025816	0.00004337	-0.00012875
Wght	0.00018314	0.00001660	-0.00001070	0.00000057
Wght	0.00017991	0.00002876	0.00001593	-0.00001632
Wght	0.00026198	0.00001619	0.00001406	-0.00001611
Wght	0.00024310	0.00004054	0.00001383	-0.00001407
Wght	0.00017693	0.23777627	-0.06754601	-0.32513793
Wght	0.00015474	0.00000545	0.00001197	-0.00001450

Figure 2.5: Jacobian Optimization Dialog Box

If you have not supplied a value for the Range, the Span is used in determining the size of the perturbation. The reason for providing the span is that it allows for better control over the perturbation which is being applied to the given variable, i.e., large enough to generate a reasonable response, without impacting the conditioning of the optimization problem (i.e., a desired very small range to work with on the variable itself).

2.7.3 Optimizer interface

While the derivative utilities are used for collecting and configuring the individual optimization objects for the problem, the Optimizer collects all of the utilities and exposes the combined list of variables and constraints to Optim. In addition, this is where you set the tolerances, flags and settings for the Optimization problem in its entirety. The Optimizer is accessed by pressing the F5 key.

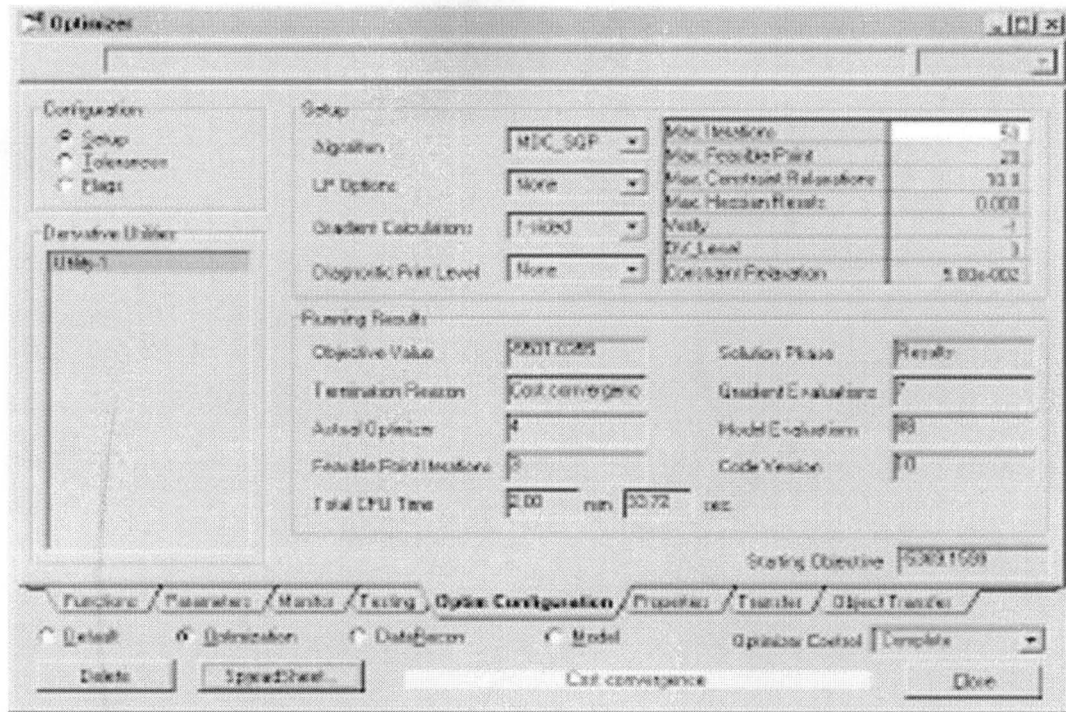


Figure 2.6: Optimizer Window

2.7.4 Optimizer configuration set up inputs (set up radio button)

These inputs consist of the following Optimizer properties and the Sequential Quadratic Programming Algorithm was selected due to its efficiency and fastness:

- Algorithm. The algorithm used by the Optimizer, is one of the following:
- SS_LP. Single-shot linear programming algorithm.
- Maximum Dual Configuration MDC_SLP. Sequential linear programming algorithm.
- Maximum Dual Configuration MDC_SQP. Two-phase sequential quadratic programming algorithm with large-scale sparse matrix handling features.
- Non Algebraic Gradient NAG_SQP. Single-phase sequential quadratic programming algorithm.

2.7.5 Gradient calculations

This option specifies if one-sided or two-sided gradient calculations are used:

- 1-sided. Causes forward differences to be used when constructing gradient approximations.
- 2-sided. Causes central differences to be used. This option requires twice as many function evaluations at a given solution, but may provide a more accurate estimate of the constraint and objective gradients, particularly for highly non-linear problems, or problems featuring large amounts of noise.

In both cases, the perturbation size used for the Optimizer internal variables is given by the Optimizer Perturbation property (www.aspentech.com.paper).

2.7.6 Maximum iterations

This parameter fulfils the following two roles:

- When Algorithm is set to MDC_SQP / MDC_SLP, this parameter gives the maximum number of Optimizer iterations allowed to improve an already feasible solution.
- When Algorithm is set to NAG_SQP, this parameter gives the maximum number of major iterations. A major iteration in this case consists of a sequence of minor iterations which minimize a linearly constrained subproblem.

2.7.7 Maximum feasible point

This parameter also fulfils two roles:

- When Algorithm is set to MDC_SQP / MDC_SLP, this parameter gives the maximum number of Optimizer iterations allowed to find the first feasible solution.
- When Algorithm is set to NAG_SQP, this parameter gives the maximum number of minor iterations. A minor iteration in this case represents a

sequence of local improvements to the linearized problem within a major iteration.

2.7.8 Maximum constraint relaxations

This parameter relates to the Relax Violated Constraints flag. This flag is used to drive the Optimizer constraint bounds to their extreme values allowed by the Optimizer tolerances. This is done to help the feasible point search part of the MDC_SQP algorithm find the first feasible solution. The Maximum Constraint Relaxations parameter gives a limit for the number of times this can occur (www.aspentech.com.paper).

2.7.9 Maximum hessian resets

The MDC_SQP algorithm operates using an approximation to the matrix of second derivatives of the objective function. On some problems, it is necessary to reset this approximation to the diagonal matrix arising from the FPS Hessian Diagonal parameter (during the FPS search) or to the diagonal matrix arising from the OPT Hessian Diagonal parameter (during the OPT search). The Maximum Hessian Resets parameter gives a limit on the number of times this can be done. This is useful if the algorithm suffers from step convergence meaning it is not used when the algorithm converges according to other criteria.

2.7.10 Verify

In the NAG_SQP algorithm, you can carry out numerical checking on gradient elements. Setting Verify to -1 switch off this checking. The extent of the numerical checking conducted by the NAG_SQP algorithm depends on the setting for Verify.

2.7.11 Termination reason

An output from the optimization run, which is one of the following:

- *OK*. Used by the FPS to indicate a feasible termination of this phase.

- *Impossible.* This output signifies either a non-implemented Optimizer algorithm is selected, or the algorithms could not find a solution to the linearized problem. In this case, the problem constraint/variable bounds and feasibility tolerance parameters should be checked.
- *No variables.* The number of variables in the problem is zero.
- *Step convergence.* During the Optimizer OPT phase of MDC_SQP, the stepping back procedure has resulted in a step collapse to below the Step solution tolerance.
- *Cost convergence.* During the Optimizer OPT phase of MDC_SQP, two successive objective function values have returned a difference in cost less than the Cost solution tolerance. Note that only feasible points are considered for this test.
- *Flat.* A special case of cost convergence in which the objective function gradient is zero. Usually indicates an incorrectly defined (or scaled) objective function.
- *Gradient convergence.* Occurs when the gradient of the Lagrangian function for the given optimization problem is less than the Gradient solution tolerance.
- *Globally infeasible.* This occurs when the feasible region cannot be seen from the FPS starting point (i.e., even the linearization of the problem does not yield a feasible solution).
- The MDC_SQP Optimizer expands the variable local bounds (the Minimum and Maximum properties of the variables) out to the global bounds (the Global Minimum and Global Maximum properties of the variables) to attempt to solve the linearized problem with these bounds. If this still yields no solution,

the FPS phase conducts a sequence of steps aimed at minimizing the constraint violations.

- An objective function is constructed which contains the sum of the constraint violations, and this function is minimized, producing a feasible solution to the problem (if one exists).
- *Infeasible*. In the Feasible Phase Sequence (FPS) phase of the optimization, if a step collapse takes place while looking for a feasible point, then the problem is considered to be infeasible due to this. This is not the same as globally infeasible.
- *Unbounded*. This occurs when the objective function is unbounded below (or is badly scaled), i.e., can be reduced without limit. This usually indicates incorrectly set constraint and/or variable bounds.
- *Time out (feasible)*. This report is generated by the OPT phase of the MDC_SQP Optimizer, when the number of Optimizer iterations during the OPT phase exceeds the Optimizer Max. Iterations parameter.
- *Time out (infeasible)*. This report is similar to the Time out (feasible) report, except occurs during the Feasible Phase Sequence (FPS) phase, when the number of iterations exceeds the Max. Feasible Point parameter.
- *Not converged*. A report solely from the NAG_SQP algorithm.
- *Not run*. Set during the Optimizer initialisation phase. This is reported in the Optimizer screen while the Optimizer is initializing.
- *Stopped*. Occurs when you stop the Optimizer using the control box on the Optimizer screen (beside the spreadsheet button) (www.aspentech.com.paper).

2.7.12 Actual optimizer

This is output from the Optimizer. It gives the number of iterations the Optimizer has conducted after finding the first feasible solution, when the MDC_SQP/SLP algorithms are used. When the NAG_SQP algorithm is used, this returns the number of major iterations used.

2.7.13 Feasible point iterations

This is output from the Optimizer. It gives the number of iterations the Optimizer has conducted in order to find the first feasible solution, again when the MDC_SQP/SLP algorithms are used. When NAG_SQP is used, this returns the number of minor iterations from the last major iteration (in this case the usefulness of this parameter is limited).

2.7.14 Solution phase

This is output from the Optimizer. It describes the current phase of the Optimizer search, which is one of:

- *Initialize*. A report that the Optimizer is initializing the diagnostics file, and preparing to carry out the Feasible Phase Sequence (FPS) search.
- *Results*. Reported when the Optimizer is writing the final solution to the diagnostics file and completing any post-optimization calculations.
- *Setup*. The Optimizer variables and constraints are being inspected and set-up internally by the Optimizer using the user-supplied data.
- *Feasible Phase Sequence*. The beginning of the FPS phase of the Optimizer.
- *Feasible Phase Sequence Deriv*. The Optimizer is calculating the gradients of the constraints and objective function during the FPS phase. This occurs every time the Optimizer adjusts the current solution to improve the feasibility of the current point.

- *Feasible Phase Sequence Visible*. The Optimizer has successfully solved the linearized problem during the FPS phase.
- *Feasible Phase Sequence Invisible*. The linearized problem at the current solution in the FPS phase cannot be solved.
- *Feasible Phase Sequence Shrink*. The Optimizer is stepping back during the FPS phase. This occurs when the projected point in the FPS is less feasible than the current point, and so the projected point is adjusted.
- *Optim*. The Optimizer is preparing to enter the FPS phase.
- *OPT Deriv*. The Optimizer is calculating the constraint and objective function gradients during the OPT phase.
- *OPT Search*. The Optimizer has successfully found a new, improved solution which remains feasible, and has moved the current solution to this point.
- *OPT Shrink*. The Optimizer is stepping back in the OPT phase. This occurs if either the projected solution is infeasible, or the objective function has increased.

2.8 Gradient Evaluations

This reports the number of gradient (constraint and objective function) evaluations during the course of the optimization. At present, this gives the correct number only when the Numerical Gradients flag is checked (www.aspentech.com.paper).

2.8.1 Model evaluations

This reports the number of plant model evaluations during the course of the optimization. At present, this gives the correct number only when the Numerical Gradients flag is checked.

2.8.2 Total CPU time

This reports the total time taken during both phases of the Optimization, in minutes and seconds.

2.8.3 Start objective

This gives the plant model cost function value at the starting point, before carrying out any optimization.

2.8.4 Perturbation

The change in the scaled variables during gradient evaluation. An individual variable in the Optimizer is scaled according to the variable Minimum property, and the variable Span property (or the *Range* property if the Optimizer Fix Variable Spans property is checked).

In general, the Optimizer scales the problem variables v to produce a set of internal scaled variables x , according to the formula.

$$X_j = \frac{V_j - Min}{S} \dots\dots\dots 2.1$$

Where Min is the variable *Minimum* property, and S is the variable Range property if the Optimizer Fix Variable Spans flag property is checked (the variable Span property otherwise). This allows equal magnitude gradients to be produced for all internal variables x , regardless of the magnitude of the external (model) variables v , by suitable choice of the variable Range properties.

The perturbation which is applied to the external variables v is therefore $\delta \times v$, where δ is the Optimizer Perturbation property (www.aspentech.com.paper).

2.8.5 FPS hessian diagonal

These give the starting values of the diagonal elements of the approximated Hessian matrices before the FPS phase of the Optimizer, of the MDC SQP algorithm.

2.8.6 OPT hessian diagonal

These give the starting values of the diagonal elements of the approximated Hessian matrices before the FPS and OPT phases of the Optimizer respectively, of the MDC SQP algorithm.

2.8.7 Jacobian elimination

The value below which entries in the Jacobian matrix are deemed to be pure model noise, and are set to zero (or when the Optimizer Sparse Jacobian flag is checked, are excluded from the Jacobian sparsity pattern and hence never re-evaluated in future).

2.8.8 Objective scale factor

This is used for scaling the objective function (and its gradient). The given function is divided by the Objective Scale Factor.

2.8.9 Major damping parameter

Used in the NAG_SQP algorithm to restrict the effects of major iteration variable moves of the scaled variables and the Lagrange multipliers. A value of 2.0 restricts the variable move to 200%.

2.8.10 Minor damping parameter

Used in NAG_SQP to restrict the effects of minor iteration variable moves. As Major Damping Parameter.

2.8.11 Penalty parameter

This is used solely in the NAG_SQP algorithm. It is used for forcing convergence of the linearized constraints solved in each NAG_SQP minor iteration to their non-linear versions which are actually evaluated in the major iterations. The larger the Penalty Parameter the slower the algorithm converges upon a feasible solution; however, this may be necessary for highly non-linear constraints (www.aspentech.com.paper).

2.8.12 Scaling type

The scaling algorithm to be used by the NAG_SQP algorithm. When set to 0, no scaling is done. Otherwise the NAG_SQP algorithm attempts to scale the Jacobian matrix in order to make the matrix coefficients as close to 1 as possible. To scale the rows only, the parameter should be set to 1. To scale the rows and columns, the parameter should be set to 2.

2.8.13 Sparse jacobian

Checked when the user wants the Optimizer to calculate the Jacobian matrix of constraint gradients in sparse form (by storing only the nonzero elements, which usually indicates constraint-variable functional dependence). This is done once, at the start of the optimization, and establishes which Jacobian elements are stored for the rest of the optimization (the sparsity pattern) (www.aspentech.com.paper).

2.8.14 Numerical gradients

Used to indicate to the Optimizer the origin of the gradient elements for the constraints and objective function.

- If the flag is checked, the Optimizer carries out numerical calculation of the gradients by direct perturbation of variables using the method specified in the Gradient Calculation flag.
- If it is unchecked, the Optimizer obtains the gradient elements from HYSYS.RTO using the same method. The main difference is that in the latter case certain gradient elements may be computed analytically, and are therefore potentially more accurate (www.aspentech.com.paper).

2.8.15 Pert_reset

Used at the start of optimization to indicate that the gradient calculation process removes noise elements (checked) or not (unchecked).

When calculating the gradient functions by perturbing Optimizer variables, model noise is introduced into the gradient elements, which can mislead the Optimizer. When v_j (perturbing variable), if it does not affect c_i (constraint), the corresponding noise can be removed from the gradients by recalculating the constraint functions after removing the perturbation from the variable.

This recalculation is done once for each variable, (i.e., for the first gradient calculation) and is used for establishing the sparsity pattern of the Jacobian matrix. The sparsity pattern is stored for use during the rest of the optimization, if the Sparse Jacobian property flag of the Optimizer is checked.

The advantages of this method are as follows:

- Removes noise terms which can mislead the Optimizer
- Does not need the Jacobian Elimination tolerance parameter, which may be difficult to set.
- Is required once only (the efficient sparse storage of the Jacobian eliminates this kind of noise from all future Optimizer steps).

The disadvantages are as follows:

- For certain models it may take much more CPU time to carry out the extra plant model evaluations, compared with the use of the Jacobian Elimination tolerance method.
- The presences of structural zeros in the Jacobian matrix are ignored. A structural zero is a forced presence of a Jacobian element, which, during first pass evaluation of the Jacobian, is zero and therefore could be excluded from the sparsity pattern.

This flag should be checked along with the Sparse Jacobian flag, since it takes advantage of the removal of model noise in terms of future computation of

gradients and their storage. However, it is still possible to use this method with a dense Jacobian matrix (where all zero elements are retained during optimization) (www.aspentech.com.paper).

2.9 Results

The results produced at the end of the optimization run are as follows:

- A price for the current model data
- Values of the Optimizer constraints and variables
- Shadow prices for the constraints and variables, if they exist
- A termination reason
- A feasibility flag for the model data at termination of the Optimizer
- Iterations taken
- CPU time taken

2.10 HYSYS.RTO Variables – Properties

The Variables in a HYSYS.RTO optimization problem are held in a Derivative Utility. This is used for holding all of the data used for defining the HYSYS.RTO Optimizer constraints and variables.

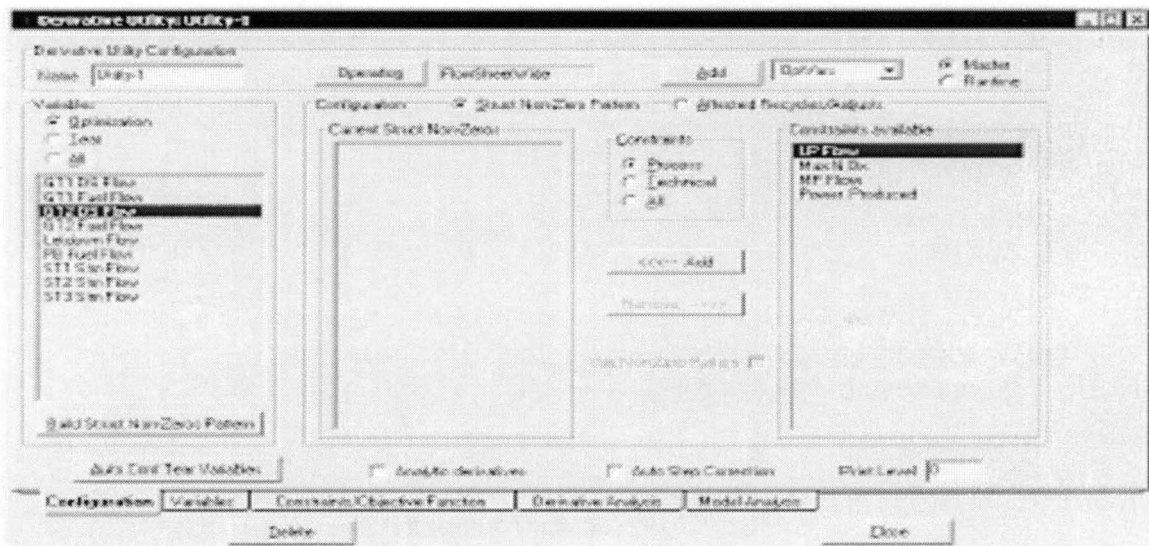


Fig 2.7: Hysys RTO Window

- The Optimizer contains a number of properties used for specifying and controlling an optimization problem for a given HYSYS.RTO case.
- The Optimizer is also associated with a Derivative Utility which contains a list of Independent Properties and Dependent Properties. The Independent Properties are the variables in the plant model that are changed to satisfy the Dependent Properties (the constraints on the plant model) simultaneously minimizing the plant model cost function (www.aspentech.com.paper).

2.10.1 Inputs variables

The configuration and Input variables (independent properties) for the derivative utility are described following the figure below:

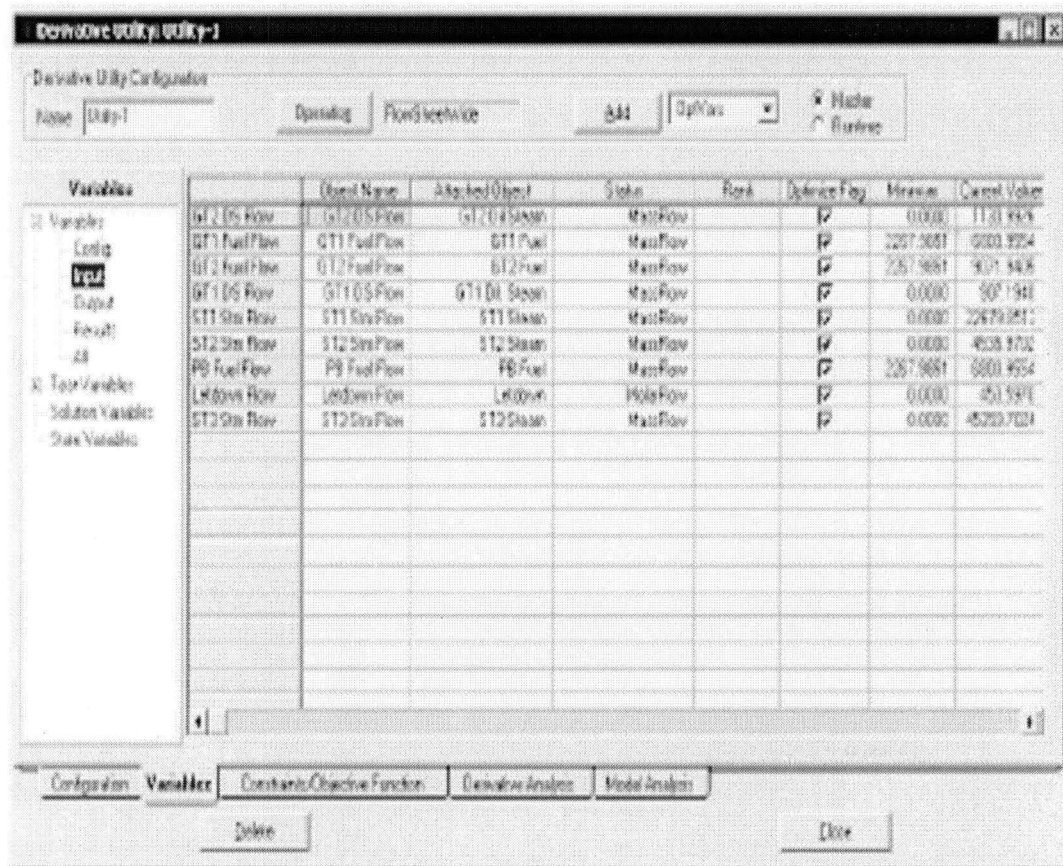


Fig 2.8: Derivative Input Variable Window

The Independent properties for Configuration and Input variables are as follows:

- *Object Name*. Name of the HYSYS.RTO object which is used as optimizer variable.
- *Attached Object*. Object (e.g., Stream or Unit Op, etc.) that is attached or associated with the listed variable.
- *Attached Property*. Property relating to the Attached Object and variable.
- *Optimize Flag*. Determines if the variable is to be used in the optimization process. If this flag is not set, no attempt is made by the Optimizer to include this variable into optimization process.
- *Minimum*. Lower bound property for the variable during the optimization process. This value might be different from its global minimum, if the change in the variable is restricted to its allowed amount, set by the maximum rate of change, during the period in the optimization process.
- *Current Value*. Current value for the property of the Object Name in the plant model.
- *Maximum*. Upper bound property for the variable during the optimization process. This value might be different from its global maximum, if the change in the variable is restricted to its allowed amount, set by the maximum rate of change, during the period in the optimization process.
- *Range*. User-specified alternative for the span. The purpose of the range is to scale the gradients of the cost function and constraints, to give similar gradient magnitudes for each variable. The gradients of the objective function (and constraints) vary inversely with the variable ranges.

- *Global Minimum.* Represents the absolute minimum value for which the variable is operated. This value is user-specified.
- *Global Maximum.* Represents the absolute maximum value for which the variable is operated. This value is also userspecified (www.aspentech.com.paper)

2.10.2 Output variables

In addition to Input variables the following variables can be seen on the Output page.

The screenshot shows the 'Derivative Utility Variable Window' with the following data:

Variable	Object Name	Applied Object	Sign	Unit	Start Value	Current Value	Unit
GT2 DS Flow	GT2 DS Flow	GT2 DS Flow	Max Flow		250.9851	111.9856	250.9851
GT1 Fuel Flow	GT1 Fuel Flow	GT1 Fuel	Max Flow		13607.9181	6803.9594	11329.5298
GT2 Fuel Flow	GT2 Fuel Flow	GT2 Fuel	Max Flow		13607.9181	6803.9594	11329.5298
GT1 DS Flow	GT1 DS Flow	GT1 DS Flow	Max Flow		250.9851	90.1940	250.9851
GT1 Sls Flow	GT1 Sls Flow	GT1 Sls	Max Flow		60029.5837	28374.2912	60029.5837
GT2 Sls Flow	GT2 Sls Flow	GT2 Sls	Max Flow		13607.9181	4525.3732	13607.9181
PG Fuel Flow	PG Fuel Flow	PG Fuel	Max Flow		8071.5405	6803.9594	6803.9594
Ledden Flow	Ledden Flow	Ledden	Max Flow		13607.9181	4525.3732	13607.9181
GT3 Sls Flow	GT3 Sls Flow	GT3 Sls	Max Flow		60029.5837	4525.3732	60029.5837

Fig 2.9: Derivative Output Variable Window

The Output variables are described below:

- *Start Value.* Starting value for the property of the Object Name in the plant model.

- *Span.* Difference between the Global Minimum and Global Maximum values for the variable and is calculated by the variable set-up. The role of the span is to convert every variable into the range (0, 1), to use uniform numerical perturbations and convergence tests.
- *Output.* Current value of the variable in the plant model. The output value is determined by the optimizer during the optimization process (www.aspentech.com.paper).

2.10.3 Results variables

In addition to the Input and Output variables, the Results variables are shown in the following figure.

Derivative Utility Configuration

Name: Utility-1 Operating Flow/Service: 644 Opt/Max Min Max

Variable	Unit	Flow	Optimize Flag	Start Value	Current Value	Status	Proc	Minimum	Maximum
GT1 [G] Flow	Flow		<input checked="" type="checkbox"/>	237.9851	111.9656	Active Low	785.891711	1.0000	237.9851
GT1 Fuel Flow	Flow		<input checked="" type="checkbox"/>	1387.9102	683.9554	Active High	4237792.2	2357.9851	1387.9102
GT2 Fuel Flow	Flow		<input checked="" type="checkbox"/>	1387.9102	9371.9405	Active High	1489158.11	2357.9851	1387.9102
GT1 [G] Flow	Flow		<input checked="" type="checkbox"/>	237.9851	907.1943	Active High	-174886.72	1.0000	237.9851
ST1 Str Flow	Flow		<input checked="" type="checkbox"/>	8809.9529	72679.8512	Active High	-212385.34	1.0000	8809.9529
ST2 Str Flow	Flow		<input checked="" type="checkbox"/>	1387.9102	4529.9122	Active High	-282715.06	1.0000	1387.9102
P0 Fuel Flow	Flow		<input checked="" type="checkbox"/>	9071.9405	683.9554	Inactive	empty	2357.9851	9071.9405
LK0 Str Flow	Flow		<input checked="" type="checkbox"/>	1387.9102	4529.9122	Inactive	empty	1.0000	1387.9102
ST3 Str Flow	Flow		<input checked="" type="checkbox"/>	8809.9529	4529.9122	Inactive	empty	1.0000	8809.9529

Configuration Variable Constants/Objective Function Derivative Analysis Model Analysis

Delete Close

Fig 2.10: Derivative Input and Output Variable Result Window

The Results variables are described below:

- *Status*. Current status of the variable, which is calculated by the Optimizer. Unlike constraints, variables are not allowed to move out of their bounds. The Status property is set to one of:
 - *Not Evaluated*. Status of the variable is not evaluated by the Optimizer.
 - *Inactive*. Variable Output property lies between the Minimum and Maximum properties, but not on one of the bounds.
 - *Equality*. Maximum and minimum properties of the variable, Minimum and Maximum, are equal, and the Output property has the same value as well.
 - *Active Low*. Variable Output property value is equal to that of the Minimum.
 - *Active High*. Variable Output property value is equal to that of the Maximum.
- *Price*. Shadow price (Lagrange multiplier) for the given variable, calculated by the Optimizer. The shadow price is used to estimate the effect which small changes to variable bounds have on the plant cost function.

The following variables are available in the All page of the Variables tree and described below.

- *Sparse Column*. Column occupied by the given variable in the Jacobian matrix. Unused variables are given a sparse column of 0.
- *Old Var Value*. Cached value of variable prior to perturbation, during gradient calculation.
- *Delta Var*. The change in variable after perturbation, during gradient evaluation.
- *Jac Offset*. The Jacobian Offset.
- *Jac Num*. The Jacobian Number.

2.10.4 Calculations

The following properties are set by the user before an optimization run:

- Global Minimum
- Global Maximum
- Range
- Start Value
- Sparse Column

The following properties are initialized by the HYSYS.RTO model before an optimization runs:

- Minimum
- Maximum
- Span

The following properties are updated by the HYSYS.RTO model during an optimization run:

- Old Var Val
- Delta Var

The following properties are updated by the Optimizer during and after an optimization run:

- Status
- Price
- Output

2.11 HYSYS.RTO Constraints – Properties

The constraints in a HYSYS.RTO optimization problem are held in a Derivative Utility and are used for holding all data used for defining the HYSYS.RTO Optimizer constraints and variables (www.aspentech.com.paper).

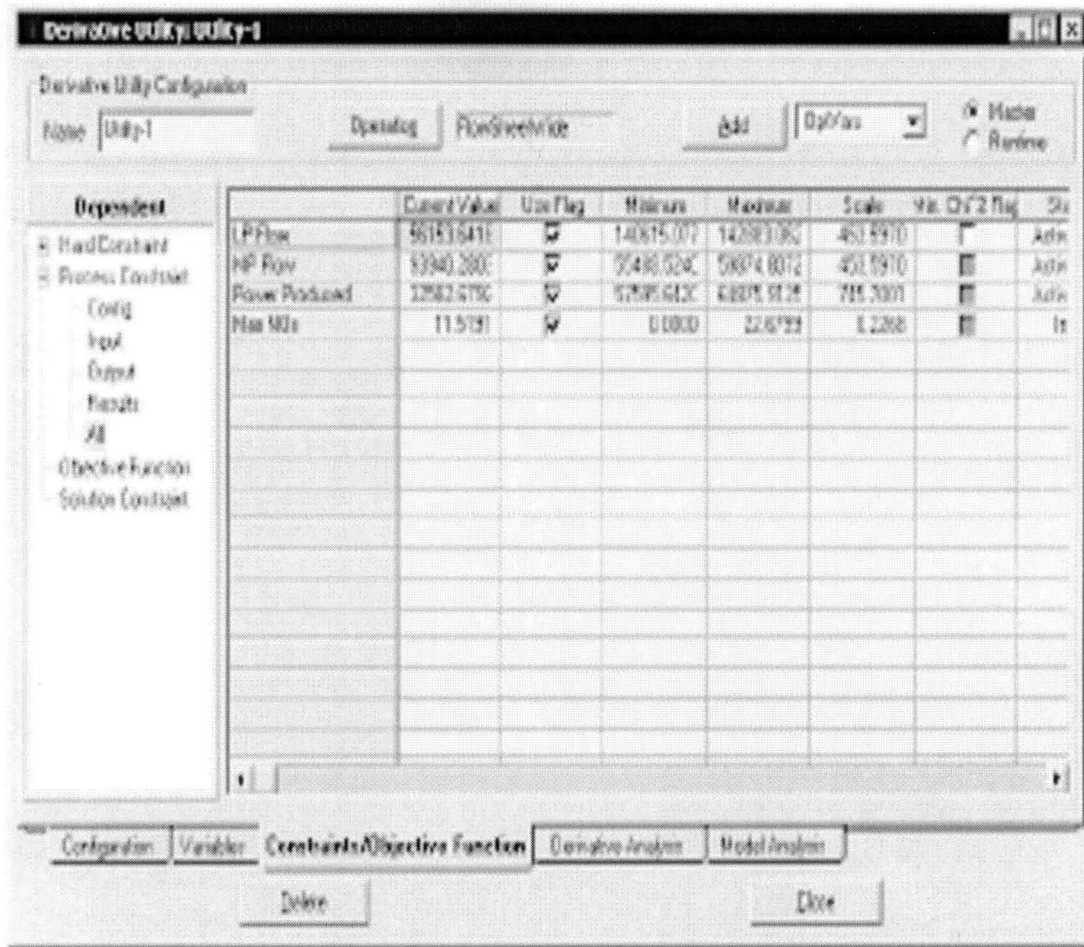


Fig 2.11: Optimizer Constraints and Variables Window

The Optimizer contains a number of properties used for specifying and controlling an optimization problem for a given HYSYS.RTO case. It is associated with a Derivative Utility that contains a list of Independent Properties and Dependent Properties. The Independent Properties are the variables in the plant model that are changed to satisfy the Dependent Properties (the constraints on the plant model) simultaneously minimizing the plant model cost function (www.aspentech.com.paper).

2.11.1 Constraint inputs

The process constraint Inputs (dependent properties) are shown on the Constraints tab below.

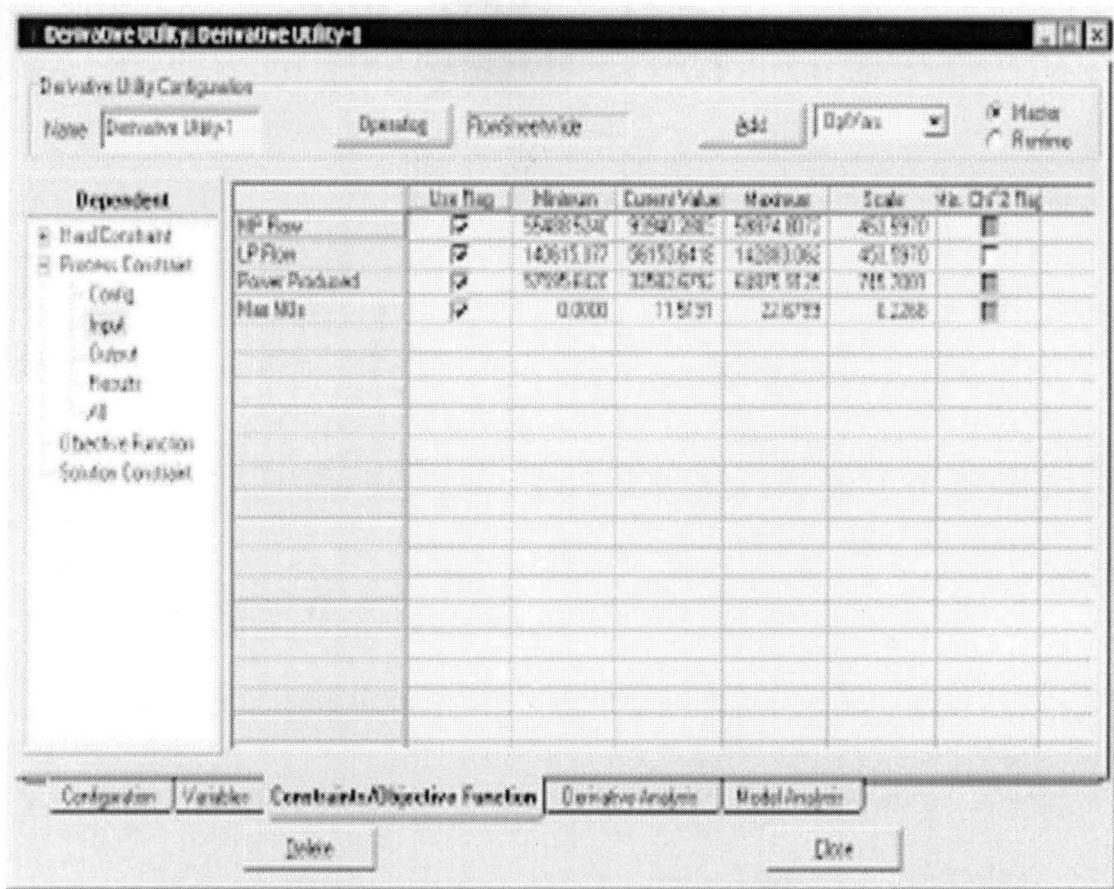


Fig 2.12: Constraints Input Window

The Dependent properties for the Configuration and Inputs process constraints are as follows:

- *Object Name.* Name of the HYSYS.RTO object to be constrained.
- *Attached Object.* Object (e.g. Stream or Unit Op, etc.) that is attached or associated with the listed variable.
- *Property.* Property related to the Attached Object and variable.
- *Current Value.* Current value for the property of the object Name.
- *Use Flag.* Determines whether the constraint is to be used in the optimization. If this flag is not set, no attempt is made by the Optimizer to satisfy this constraint.
- *Minimum.* The lower bound for the constraint, which is user-specified.

- *Current*. Current value the constraint possesses in the plant model.
- *Maximum*. The upper bound for the constraint, which is also user-specified.
- *Scale*. A user-supplied number that gives the scale on which the feasibility of the constraint is measured. This property is used in conjunction with the Optimizer Zeta property, which is a relative feasibility tolerance. In general, a constraint is said to be feasible if:

$$\text{Minimum} - \text{Scale} \times \text{Zeta} \leq \text{Currents} \leq \text{Maximum} + \text{Scale} \times \text{Zeta}$$

- Where Minimum and Maximum are the lower and upper bound properties respectively, of the constraint, and Current is its current value (equivalent to Hooked Property for constraints which have the Use Flag checked).
- *Minimum Chi Square*. Determines whether or not a chi-square test is done for the constraint (www.aspentech.com.paper).

2.11.2 Constraints outputs

The process constraint Outputs (dependent properties) are shown on the Constraints tab below.

Constraint	Current Value	Status	Normalization	Base Value	Price
LP Flow	56143.6411	Active Low	50000.0000	143576.377	54.8858
HP Flow	83540.2808	Active Low	50000.0000	55431.4754	45.1461
Power Produced	22582.6756	Active Low	10000.0000	57058.8314	8.2280
Heat MBs	11.5781	Inactive	0.4548	20.1082	empty

Fig 2.13: Process Constraint Outputs

The Dependent properties for the Output process constraints are as follows:

- *Status*. The current status of the constraint, which is calculated by the Optimizer. The Status property is set to one of:
 - *Not Evaluated*. The status of the constraint has not been evaluated by the Optimizer.
 - *Inactive*. The constraint Current property lies between the Minimum and Maximum properties, but is neither Active High nor Active Low.
 - *Violated Low*. The constraint Current property is less than $\text{Minimum} - \text{Scale} \times \text{Zeta}$, where Scale is the constraint Scale property and Zeta is the Optimizer Zeta tolerance property.
 - *Violated High*. The Current property is greater than $\text{Maximum} + \text{Scale} \times \text{Zeta}$.
 - *Active Low*. The constraint Current property is less than $\text{Minimum} + \text{Scale} \times \text{Zeta}$, but greater than $\text{Minimum} - \text{Scale} \times \text{Zeta}$.
 - *Active High*. Constraint current property is greater than $\text{Maximum} - \text{Scale} \times \text{Zeta}$, but less than $\text{Maximum} + \text{Scale} \times \text{Zeta}$.
- *Normalization*. When the Jacobian matrix is first calculated (first pass evaluation) the Normalization property for the constraint is set to be the largest Jacobian entry in the row (Sparse Row) of the Jacobian matrix corresponding to this constraint. This number is used to normalize the rest of the given Jacobian row, for all remaining Optimizer search steps (i.e., is not recalculated).
- *Base Value*. When calculating the gradient of a given constraint with respect to each variable, the internal scaled variable is perturbed away from the current point by adding the number specified in the Optimizer Perturbation property. The new value of the constraint is found corresponding to the new

variable value, and the change in constraint, divided by the change in the variable, is the corresponding Jacobian element.

- The constraint Base property stores the pre-perturbation value of the constraint. Under certain circumstances, however, the Base property itself can change during the Jacobian calculation. This is due to the fact that removing a perturbation from a perturbed variable, and re-running the plant model, will not reproduce the previous Base property within the constraint Current property; this is due to noise in the model arising from non-zero convergence tolerances (i.e., the un-perturbed constraint Current differs slightly from the pre-perturbed Current).
- Therefore, under certain circumstances (when the Pert_Reset flag property of the Optimizer is checked) the Optimizer will remove the perturbation from the variable, re-run the plant model, and then re-set the Base property of the constraint to match the re-calculated Current property. This eliminates associated noise from the Jacobian matrix. This method is discussed in more detail in the Optimizer Properties document [3], in the Pert_Reset section.
- *Price*. Shadow price (Lagrange multiplier) for the given constraint, calculated by the Optimizer. If a feasible solution is found by the Optimizer, then a simple interpretation of the Lagrange multiplier is that it gives the gradient of the cost function along the corresponding constraint normal. Thus, the shadow price indicates the approximate change to the objective function when increasing (i.e., relaxing) the given active bound by a unit amount (www.aspentech.com.paper).

2.11.3 All constraints

The following constraints can be found on the all page of the Process Constraint, Dependent properties tree.

- *Hard Constraint*. User-specified flag that indicates whether the constraint is a technical one, i.e., is a process specification such as a mass balance or a temperature, as opposed to purely an economic constraint.
- *Off Flag*. User-specified flag that indicates whether the constraint is in the 'off' state, or not. This is often used when related items of equipment are being constrained, which themselves have an on-off behaviour.
- *Sparse Row*. Number of the row in the Jacobian matrix which is occupied by the given constraint.
- *Old Cons Value*. Value of the constraint prior to perturbation of a variable, during gradient calculation.
- *Bias1*
- *Delta Cons*. Change in constraint after perturbing a variable, during gradient evaluation.

2.11.4 Calculations

The following properties are updated by the HYSYS.RTO model during an optimization run:

- Base Value
- Old Cons Val

The following properties are updated by the Optimizer during and after an optimizations run:

- Status
- Normalization

- Price
- Sparse Row
- Current

CHAPTER THREE

3.0 METHODOLOGY

The optimization of Crude Distillation Column was carried out using Hysys simulation software. The procedure for carrying out the task involves process simulation of the CDU (Base Case) and process optimization respectively. Hysys simulation software was used to carry out the two tasks. The procedure for both process simulation and process optimization are described below.

3.2 Process Simulation Procedure

The procedures for the simulation of the crude distillation column are described below:

1. The Hysys Package was launched and the Basis Environment was entered then Oil Manager was selected and Oil Environment was viewed.
2. Under the Cut/Blend tab, the default crude blend was selected and the View button was clicked.
3. The Tables tab was opened. This is where the information was displayed.
4. The Oil Distributions Table Type and the Straight Run cut option were used, for the characterization of the crude oil.
5. A material stream named Btm Steam was created with the following parameters namely temperature, pressure and flow rate as shown in figure 3.1:

Table 3.1: The Bottom Specification

Item	Enter
Name	Bottom
Vapour Fraction	1
Pressure	1380 kPa
Flow	3400 kg/hr

6. The Atmospheric Column was simulated as a Refluxed Absorber.
7. The Refluxed Absorber icon was selected.
8. The Input Expert for The Refluxed Absorber is displayed below in Table 3.2:

Table 3.2: Refluxed Absorber Icon (Chiyoda, 1980).

Item	Enter...
Column Name	Atmos Tower
# Stages	29
Inlet Stream	ATM Feed
Inlet Stage	28_Main TS
Bottom Stage Inlet	Btm Steam
Stage Numbering	Top Down
Condenser Energy Stream	Cond Duty
Condenser	Partial
Overhead Outlets	Off Gas Naphtha
Condenser	Partial
Bottoms Liquid Outlet	Atm Residue

9. The Water Draw checkbox was checked and the stream Waste Water was named.

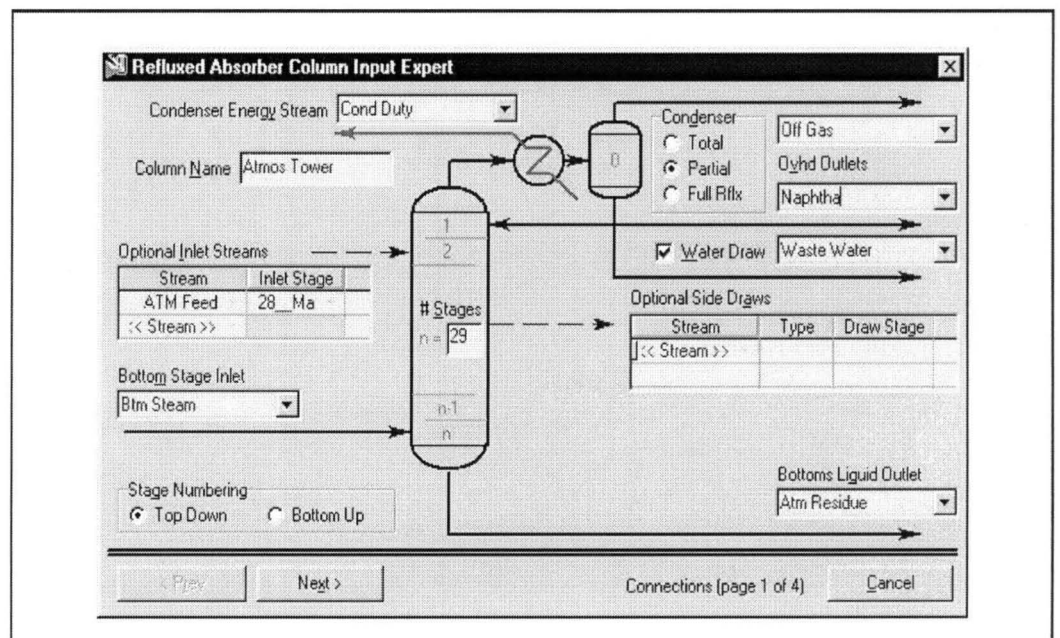


Figure 3.1: Reflux Absorber Column Input Expert

9. The next page of the Input Expert was Moved to and the data in Table 3.3 below were Entered:

Table 3.3 Refluxed Absorber Input Data (Chiyoda, 1980).

Item	Enter
Condenser Pressure	140.0 kPa (20.31 psia)
Condenser Pressure Drop	60.00 kPa (8.7 psi)
Bottom Stage Pressure	230.0 kPa (33.36 psia)

10. The pressure for the stage 1 in the crude column was provided and the column Converged as shown in Figure 3.2

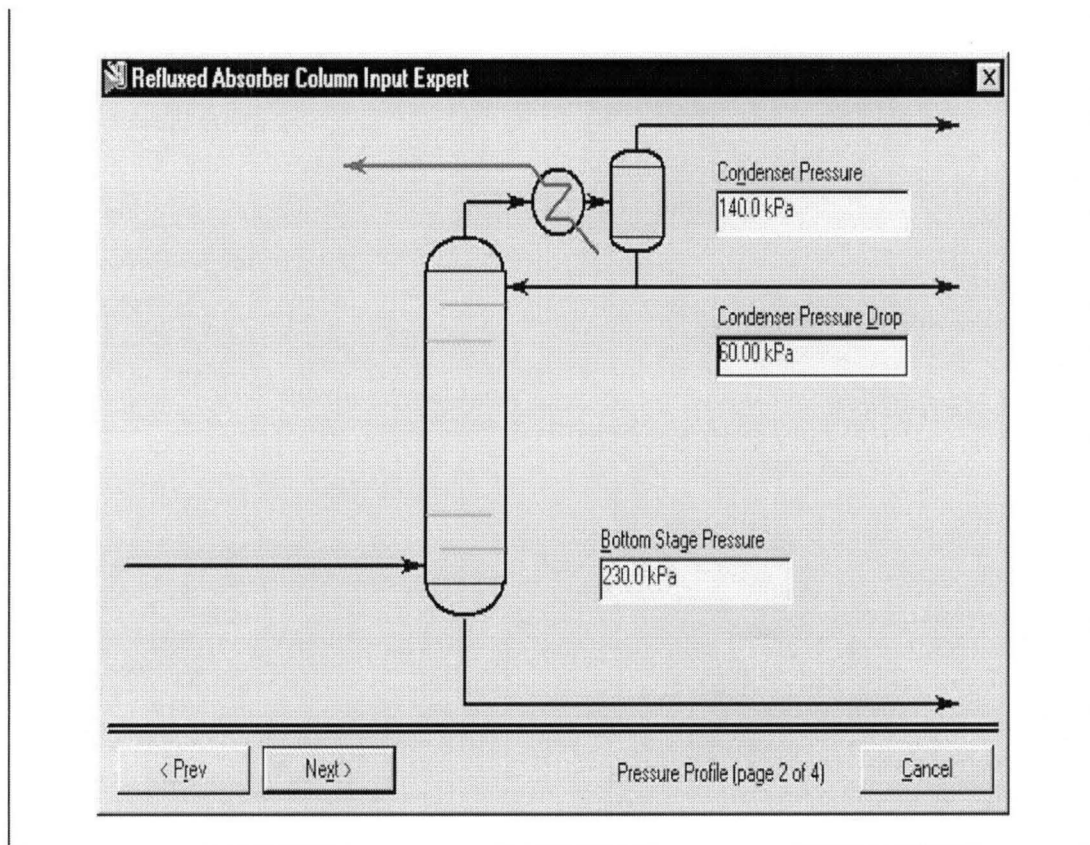


Figure 3.2: Reflux Absorber Column Input Expert

11. The next page of the Input Expert was moved to and the data were entered as shown in Figure 3.3

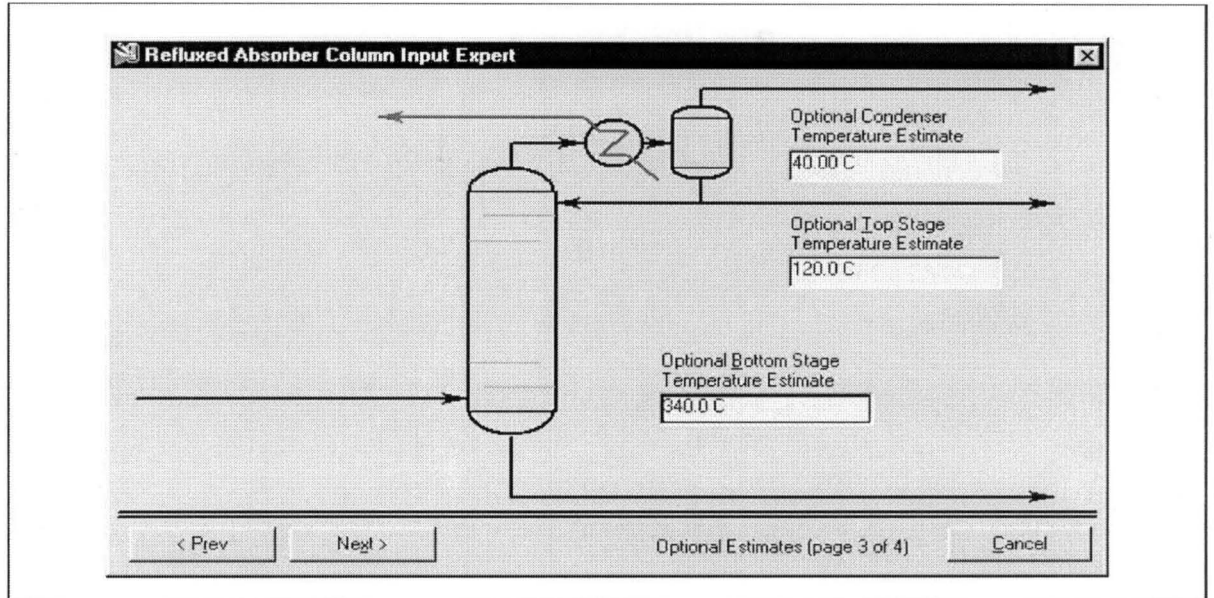


Figure 3.3: Reflux Absorber Column Input Expert

12. The next screen of the Input Expert was moved to and 0 kgmole/h was entered (Chiyoda, 1980) in the Vapour Rate field as shown in Figure 3.4

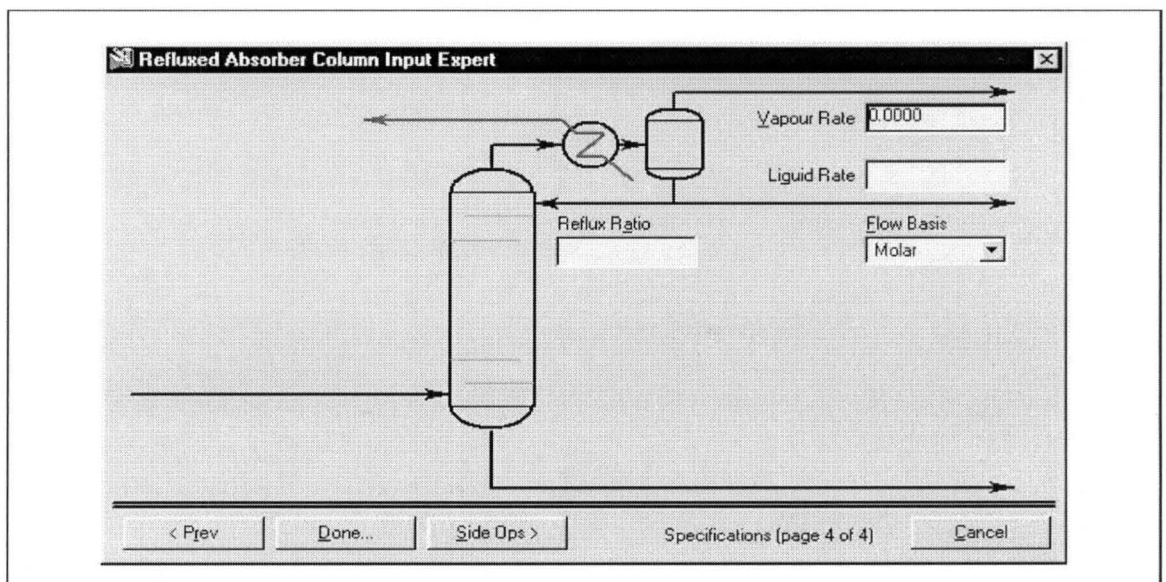


Figure 3.4: Reflux Absorber Column Input Expert

13. The Done button was clicked, and Column Property View was placed. Then the Design tab was moved to and the Monitor page was opened.
14. A Distillate Rate of $150 \text{ m}^3/\text{h}$ was specified, the property view was opened and the Flowrate type was also changed.
15. The Vap Prod Rate basis was activated.
16. The default spec of Reflux Ratio was deactivated, then the Degrees of Freedom was set to 0 and the column converged (Chiyoda, 1980).
15. The Run button was clicked and the column converged.

Adding the Side Strippers and the Pump Arouns

16. The Side Ops tab was used and the Side Ops Input Expert button was clicked.
17. The Next button was clicked once to move to the appropriate input expert.
18. The Add Side Stripper button was Clicked, and
19. The Install button was Clicked and the side stripper and associated streams to the Simulations were added by HYSYS.
20. The Next button was clicked twice and the appropriate input expert selected.
21. The Add Pump Around button was clicked and the operation was added.
22. The Install button was clicked and the operation was added to the simulation.
23. The Side Ops Input Expert view was closed and the Monitor page of the Design tab was returned to.
24. The following three specifications were added (AGO Side Stripper Product Flow, AGO PA Rate and AGO PA Duty):
25. HYSYS automatically creates four specifications when the side operations are added via the input expert.
25. The specified value for the specifications were selected and made active.

26. The following values for the various specifications were used. (AGO SS Prod Flow = 30 m³/h, AGO PA Rate = 200 m³/h and AGO PA Duty = -3.7E7 kJ/h) respectively.

27. The specifications in tables 3.4 and 3.5, below were entered as shown in figures 3.5 and 3.6 respectively.

Table 3.4 Side Operations Input Data

Item	Enter
Name	AGO SS
Return Stage	21_Main TS
Draw Stage	22_Main TS
Steam Feed	AGO Steam
Draw Product	AGO Prod

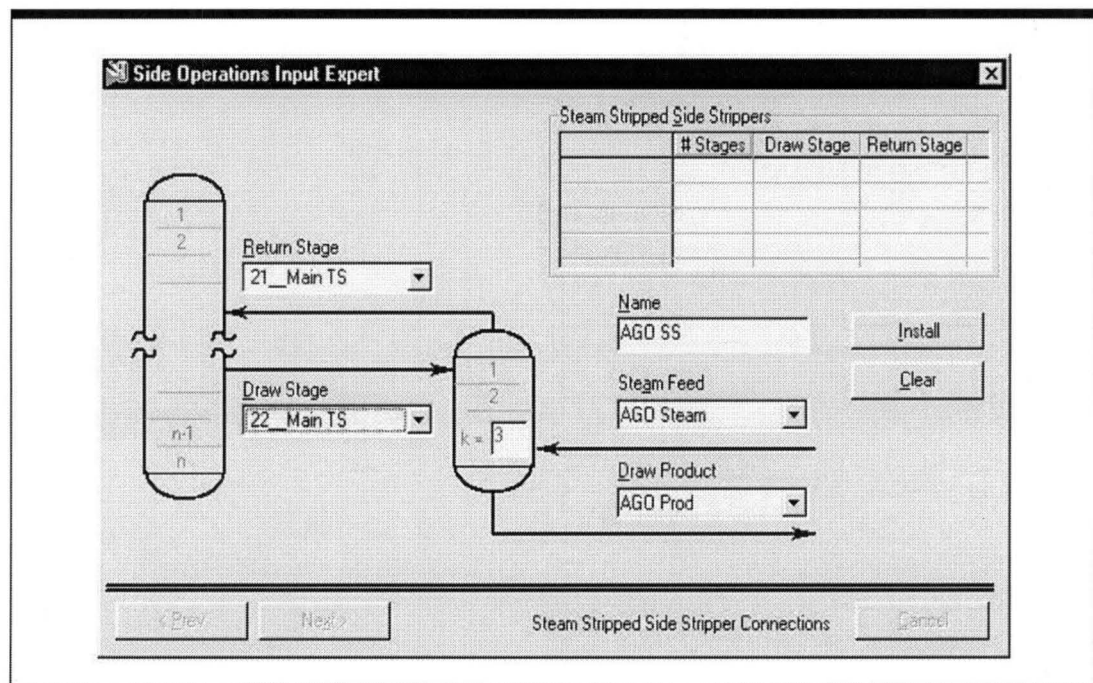


Figure 3.5 Side Operations Input Expert

Table 3.5 Side Operations Input Data

Item	Enter
Name	AGO PA
Return Stage	21_Main TS
Draw Stage	22_Main TS

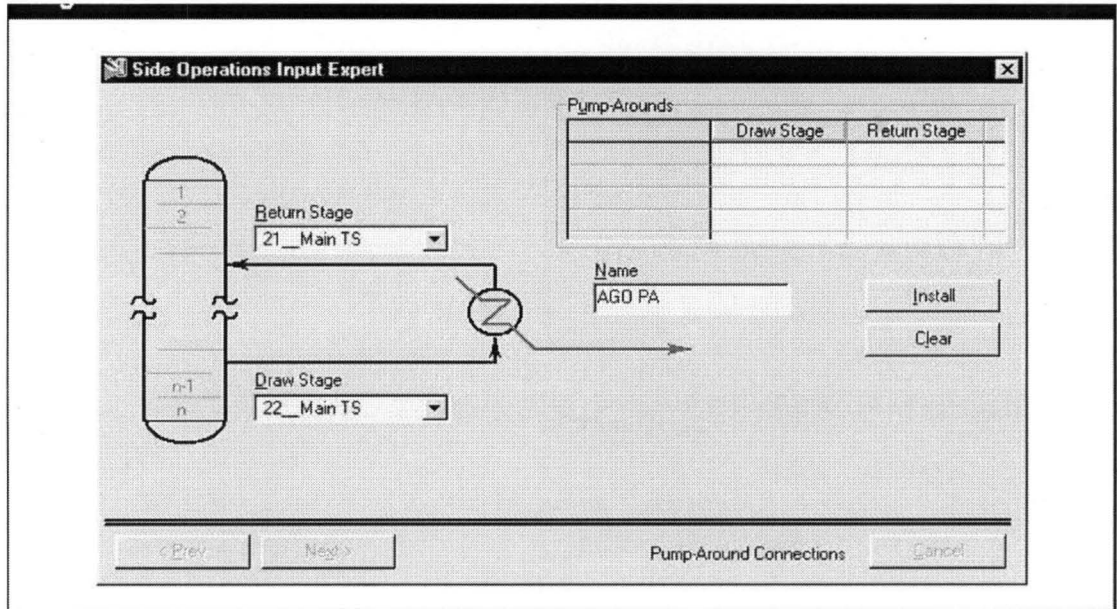


Figure 3.6 Side Operations Input Expert

28. The Reset icon was clicked and the specified values activated and the column converged.
29. The data were entered On the Work Sheet tab for the AGO Steam stream:
30. The Design tab and Monitor page were Returned to and the Degrees of Freedom was set to 0.
31. The Run button was clicked and the column converged.
32. The Column Environment was entered and the Side Stripper was selected on the Side-Ops tab, then the Add button was clicked and the information in Table 3.6 below was entered.

Table 3.6 Side Operations input data (Chiyoda, 1980).

Item	Enter
Name	Diesel SS
Return Stage	16
Draw Stage	17
Flow Basis	Volume (select this radio button)
Product Stream	Diesel Prod
Draw Spec	130 m ³ /h (19,250 bbl/d)
Configuration	Steam Stripped
Steam Feed	Diesel Steam

33. The Install button was clicked and the view was closed

34. The Pump Arouns was selected On the Side Ops tab and the Add button was clicked and the following information were entered.

Table 3.7 Pump Arouns Input Data

Item	Enter
Name	Diesel PA
Return Stage	16
Draw Stage	17

36. The Work Sheet tab was clicked and the following information were entered for the Diesel Steam stream:

Table 3.8 Diesel Steam Stream Side Operations Input Data (Chiyoda, 1980).

Variable	Values
Temperature	150°C
Pressure	350 kPa
Mass Flow	1350 kg/h
Composition	100% H ₂ O

37. The Design tab and Monitor page were Returned to and the Degrees of Freedom was set to 0 (Chiyoda, 1980) .

38. The Run button was clicked the column converged.

39. Another Side Stripper was added with the following information:

Table 3.9 Kerosene stream Side Operations input data

Item	Enter
Name	Kerosene SS
Draw Stage	9
Return Stage	8
Prod Stream	Kerosene Prod
Prod Rate	62 m ³ /h
Configuration	Reboiled
Boil Up Ratio	0.75

40. A third Pump Around was added.
41. The Design tab and Monitor page was returned to and the Degrees of Freedom was set to 0 (Chiyoda, 1980).
42. The Run button was clicked and the column converged.
43. The Process Flow Diagram (PFD) in the parent environment was entered and a new Energy stream was created and named Trim Duty and no duty *were* specified for this stream.
44. The column was Double-clicked and the Connections page on the Design tab was Clicked. Then the Inlet Streams group was clicked and the Trim Duty stream in a new External Stream cell was added, and stage 28 was specified as the feed stage (Chiyoda, 1980).
45. The Monitor page was entered and the Add Spec button was clicked in the Specification group.
46. The Column Liquid Flow was Chosen from the list that appears and the Add Spec button was clicked.
47. The data were entered and the specifications were made active.
48. The Kerosene SS BoilUp Ratio specification was changed to an Estimate only.

49. A Column Duty specification of (7.5e6 Btu/hr) was entered as shown in Figure 3.7.

50. The Monitor page was returned to and the degree of Freedom was set to 0 (Chiyoda, 1980).

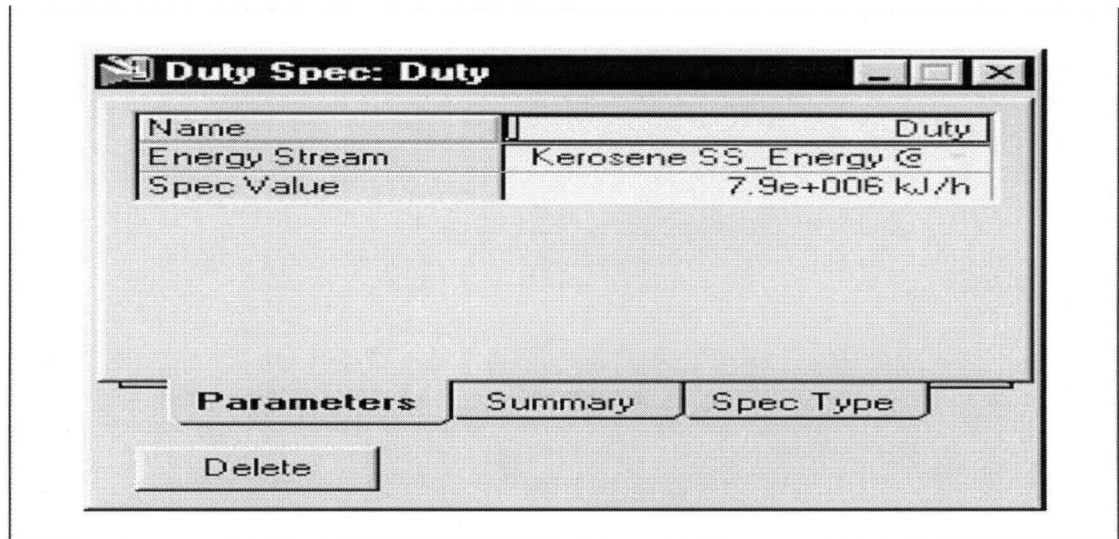


Figure 3.7 Duty Specification for Kerosene Side Stripper

51. The Run button was clicked the column converged

3.3 Process Optimization Procedure

1. The simulation case was loaded from the Atmospheric Crude Distillation Column
2. From the Tools menu, Preferences was selected.
3. The Variables tab was clicked and the Units page was selected.
4. The Refinery package was selected.
5. The cursor was moved to the Energy cell and the Add button was clicked.
6. The view was completed as shown in Figure 3.8

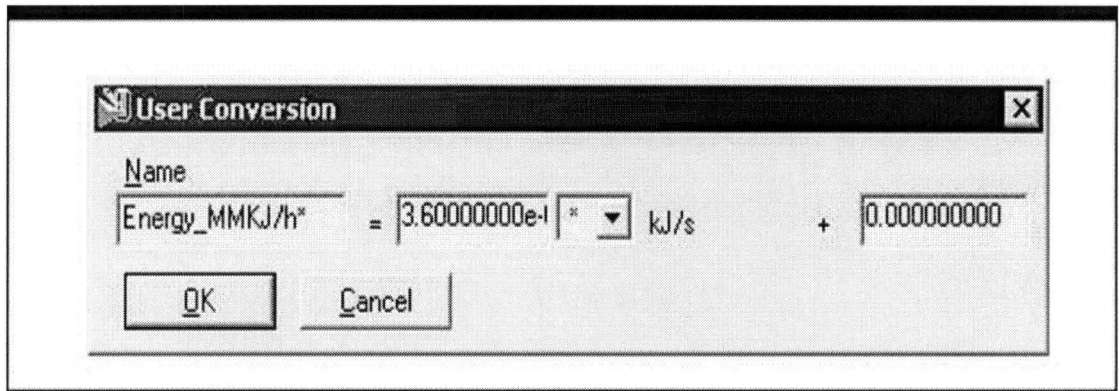


Figure 3.8 User Conversion in Hysys Environment

7. The Column Property View was Opened.
8. The feed Temperature was Changed to 320°C.
9. The Design tab was Clicked and then the Monitor page was clicked.
10. The Kerosene flowrate was Entered as 62 m³/h. and the specifications on the Monitor page appears as shown in Figure 3.9 below.

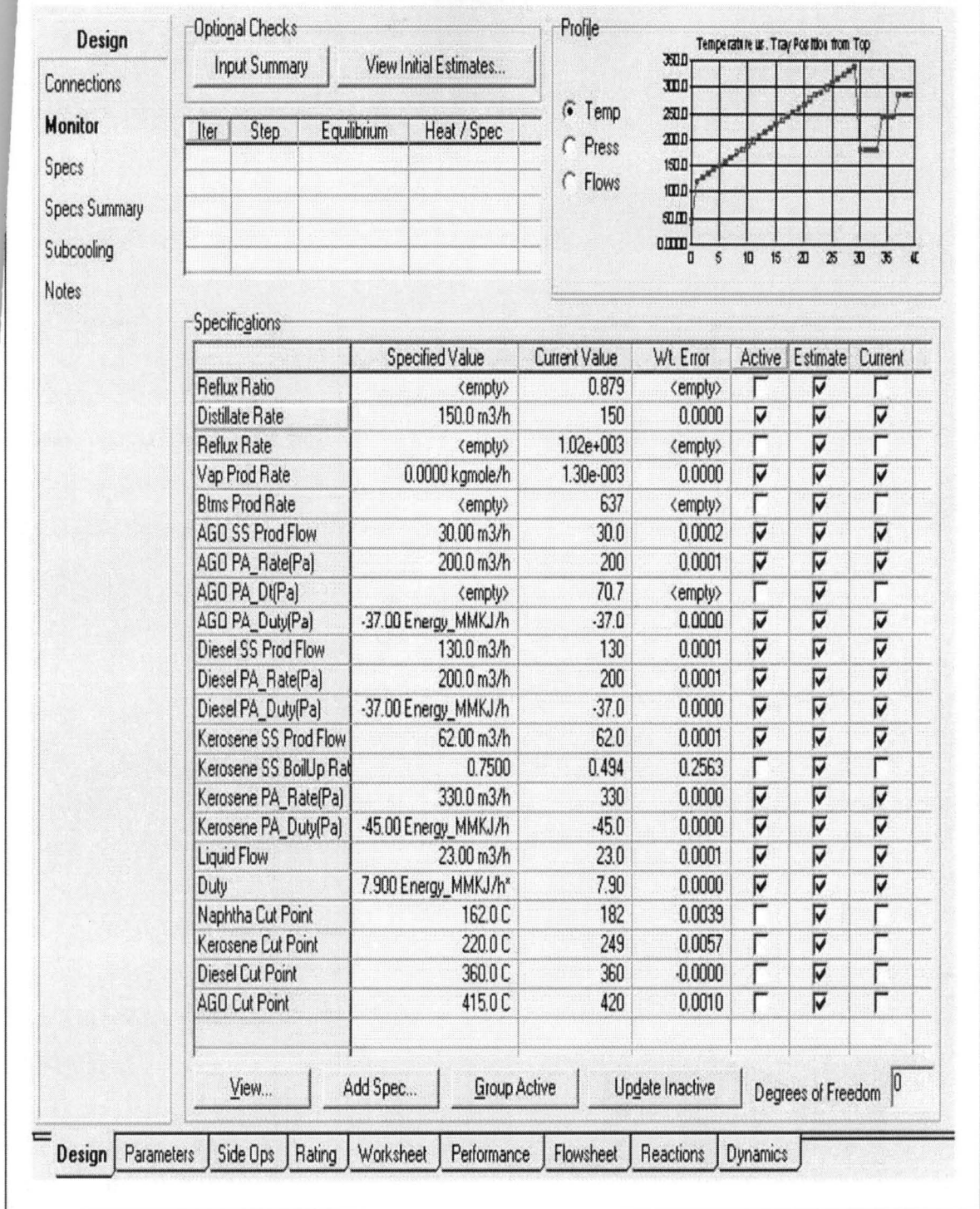


Figure 3.9 Specifications Monitor for the Distillation Column Side Stripper

11. From the Tools menu, Utilities was selected.
12. Derivative Utility was clicked in the list box on the right.
13. The Add Utility button was Clicked and The Derivative Utility property view appears as shown in Figure 3.10

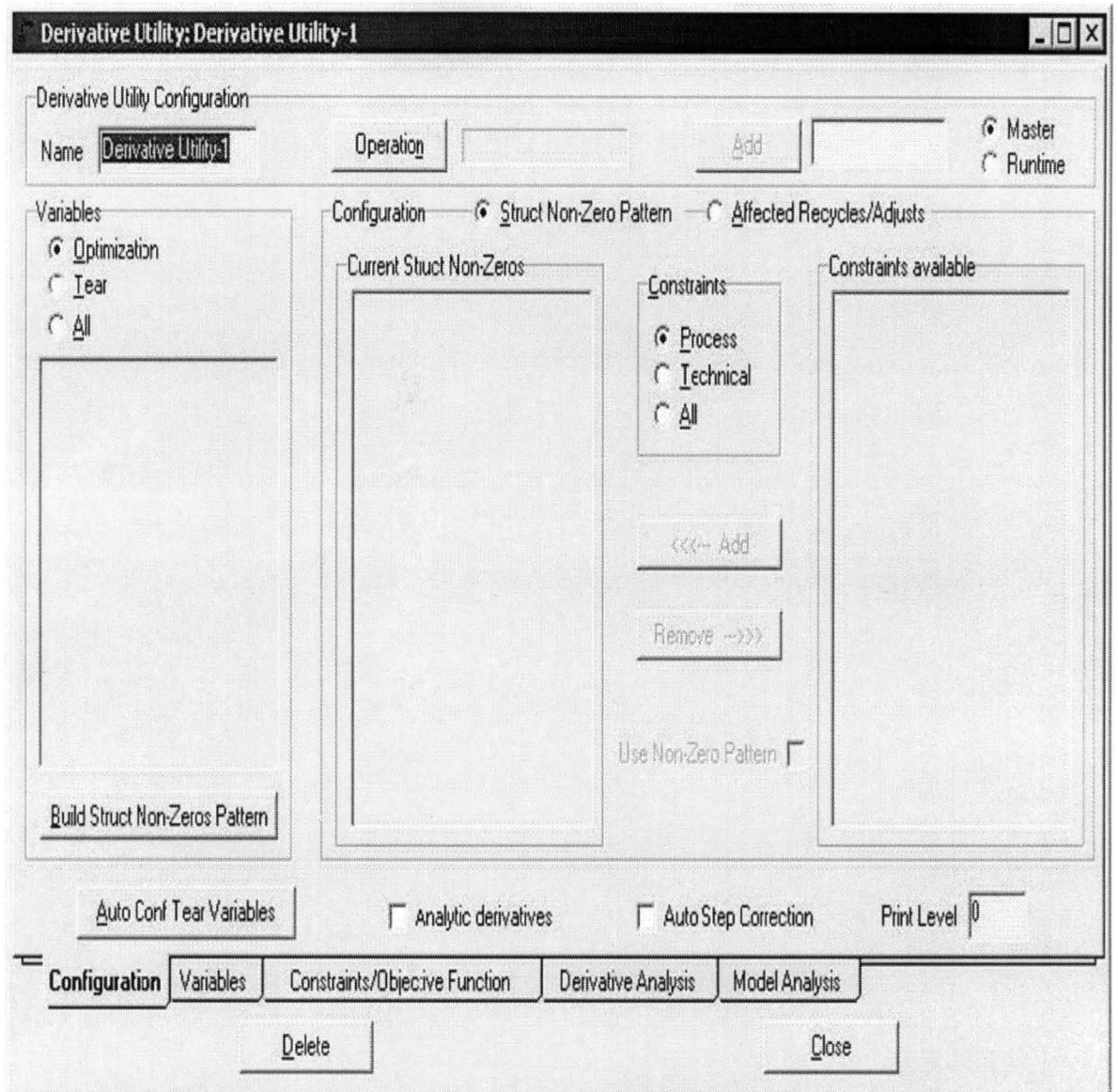


Figure 3.10 Derivative Utility Properties for the Distillation Column

14. The Operation button was clicked.

15. The Atmos Tower was added to the Scope Objects list as shown in Figure 3.11 below

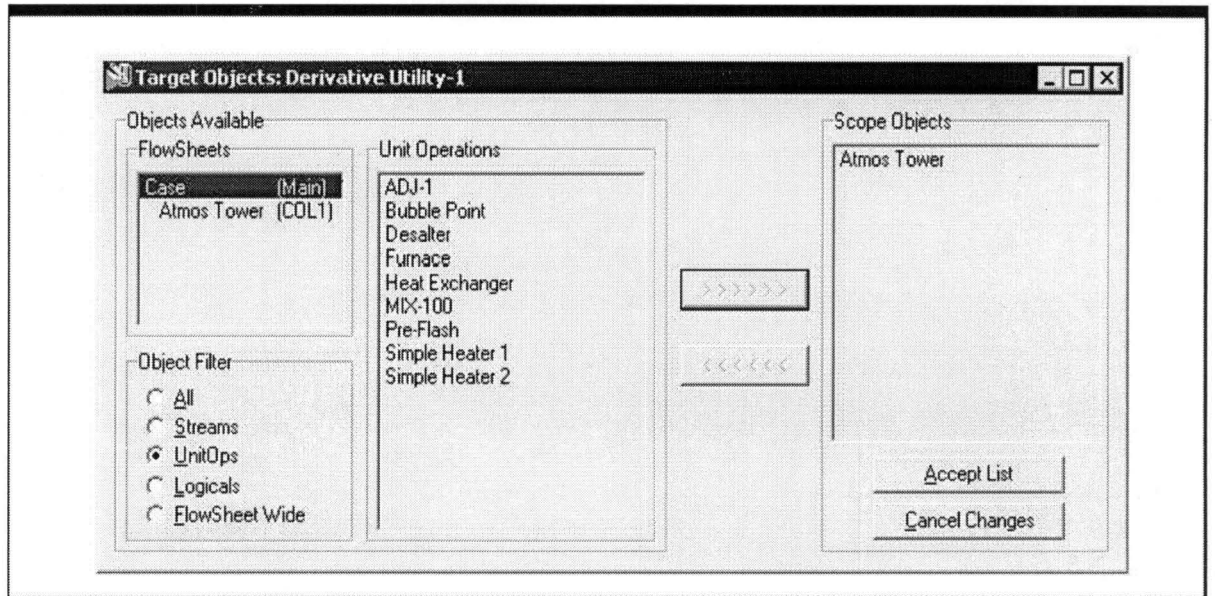


Figure 3.11 Target Objects Addition derivative Utility

16. Accept List was clicked.

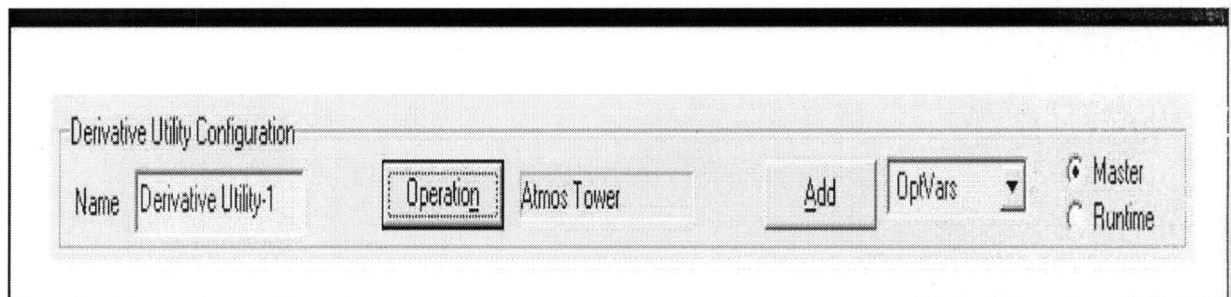


Figure 3.12 Derivative Utility Configuration

17. OptVars was Selected and the Add button to the left of the drop-down list

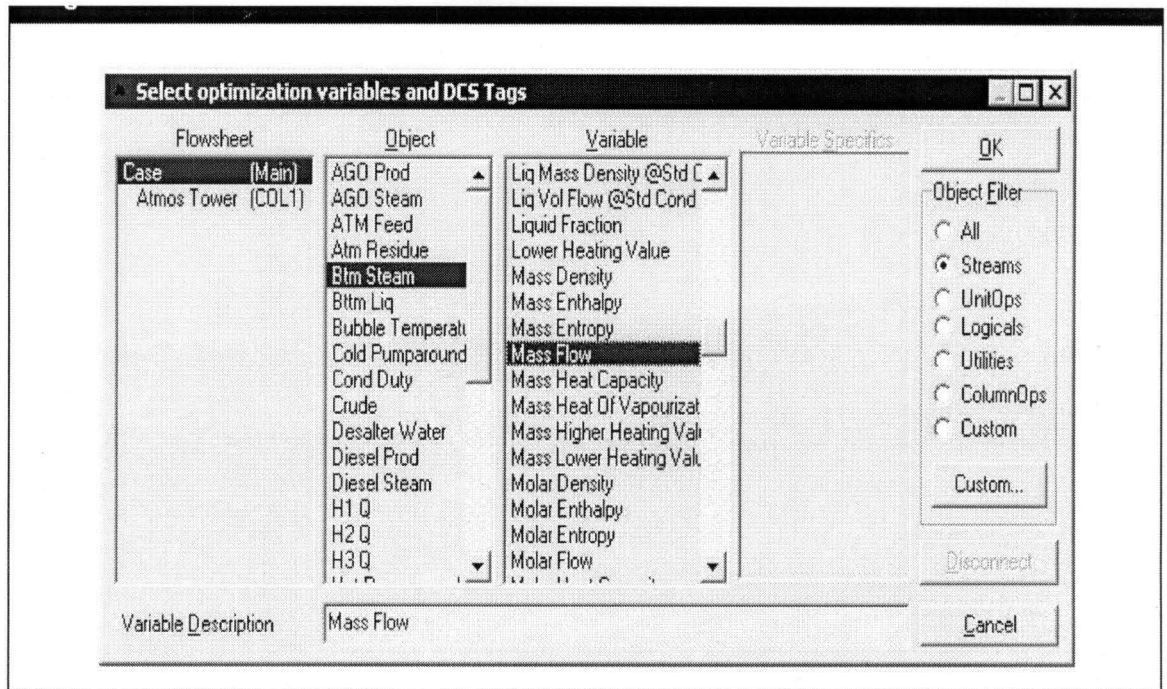


Figure 3.13 Select optimization and DCS Tags View

18. The Add button was Clicked and the OptVars option was selected in the drop-down list.

19. The steam flowrates were added.

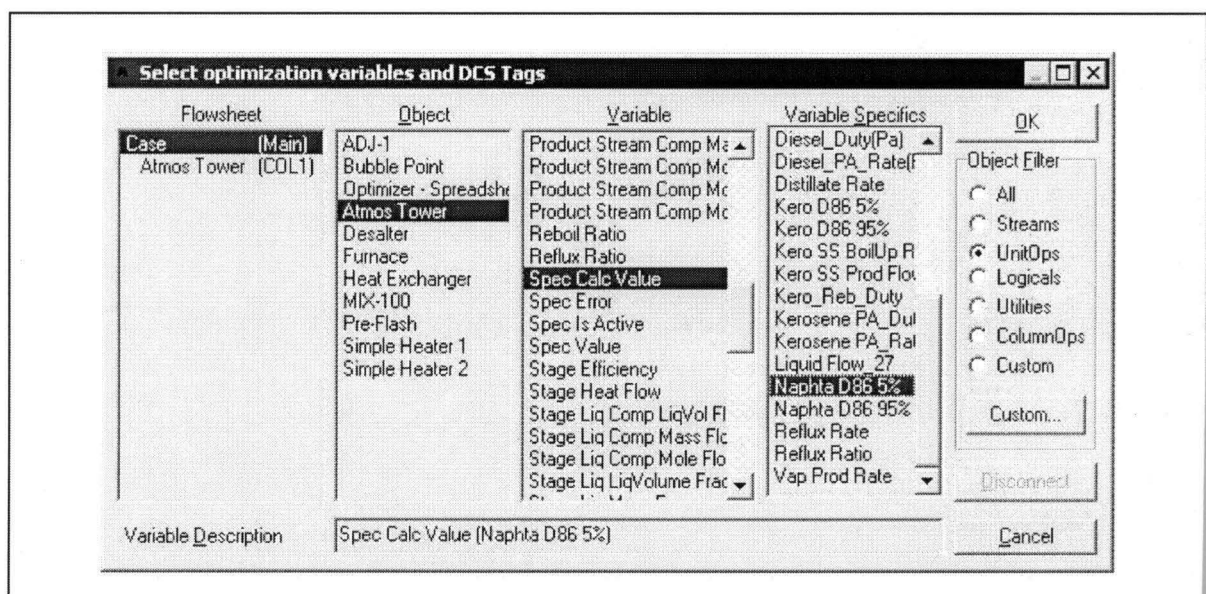


Figure 3.14 Optimization Variables Selection View

20. The steps were Repeated in order to complete the list of Optimization variables as shown below:

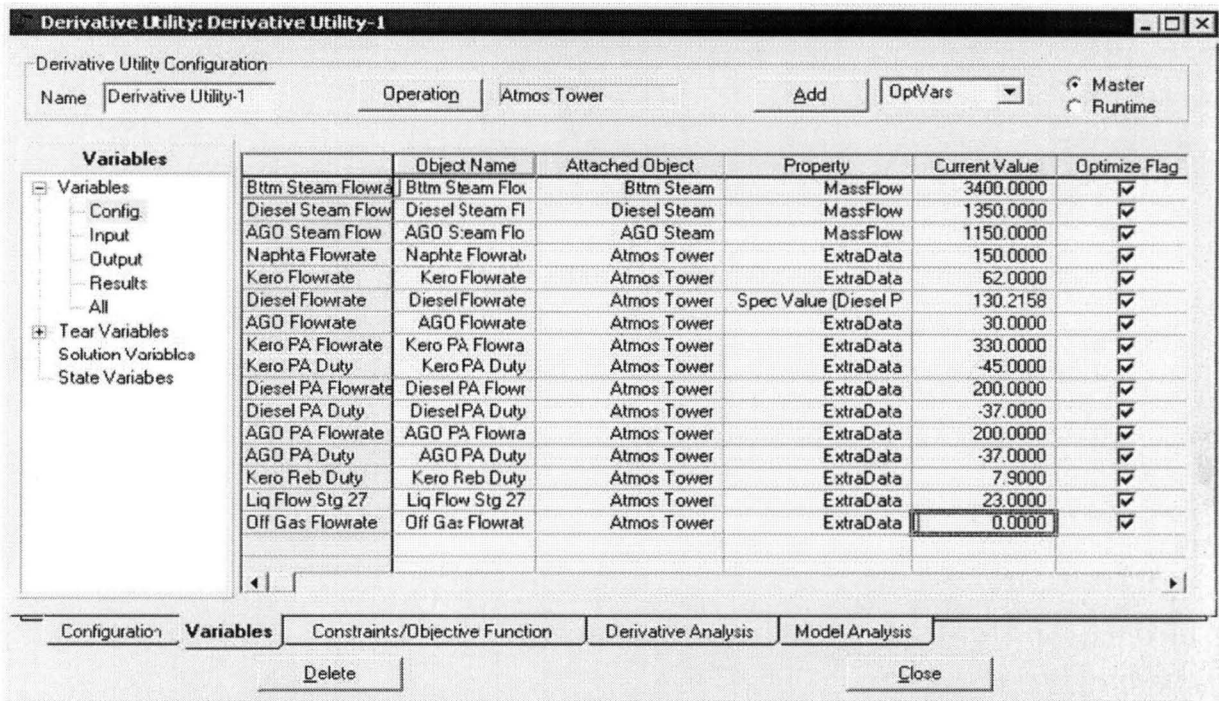


Figure 3.15 Select optimization and DCS Tags View

21. The Input view was selected from the Variables tree on the left.

22. The minimum and maximum values for each of the variables were Completed.

23. The Add button was Clicked and the ProcCons option was activated in the drop-down list as shown in Figure 3.16

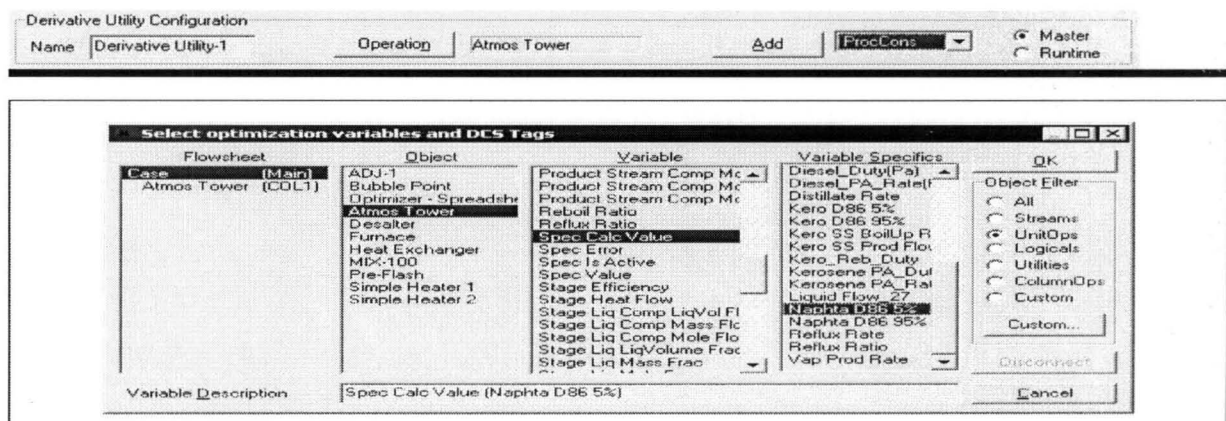


Figure 3.16 Select optimization Variables configuration

Table 3.10 Maximum and Minimum Temp. values for the optimization variables

Item	Specification type	Minimum (°C)	Maximum (°C)
Naphtha	D86 / 5%	40.00	50.00
Naphtha	D86 / 95%	160.00	180.00
Kerosene	D86 / 5%	170.00	190.00
Kerosene	D86 / 95%	240.00	260.00
Diesel	Pour point	-15.00	5.00
Diesel	Flash point	90.00	110.00
AGO	Pour point	0.00	20.00
AGO	Flash point	130.00	150.00

24. The steps were repeated in order to complete the whole list of Constraint variables as displayed in the previous table.
25. For the heavy streams, Flash Point and Pour Point specifications were included by selecting them from the column.
26. The Monitor page was entered.
27. The Add Spec button was clicked.
28. The Add Spec button was clicked again and the Cold Properties were selected.
29. The equipment limitation constraints were taken into account.
30. Two new process constraints for the Energy streams were added.
31. To add Objective Function variables, the Add button was clicked and the ObjFunc option selected.

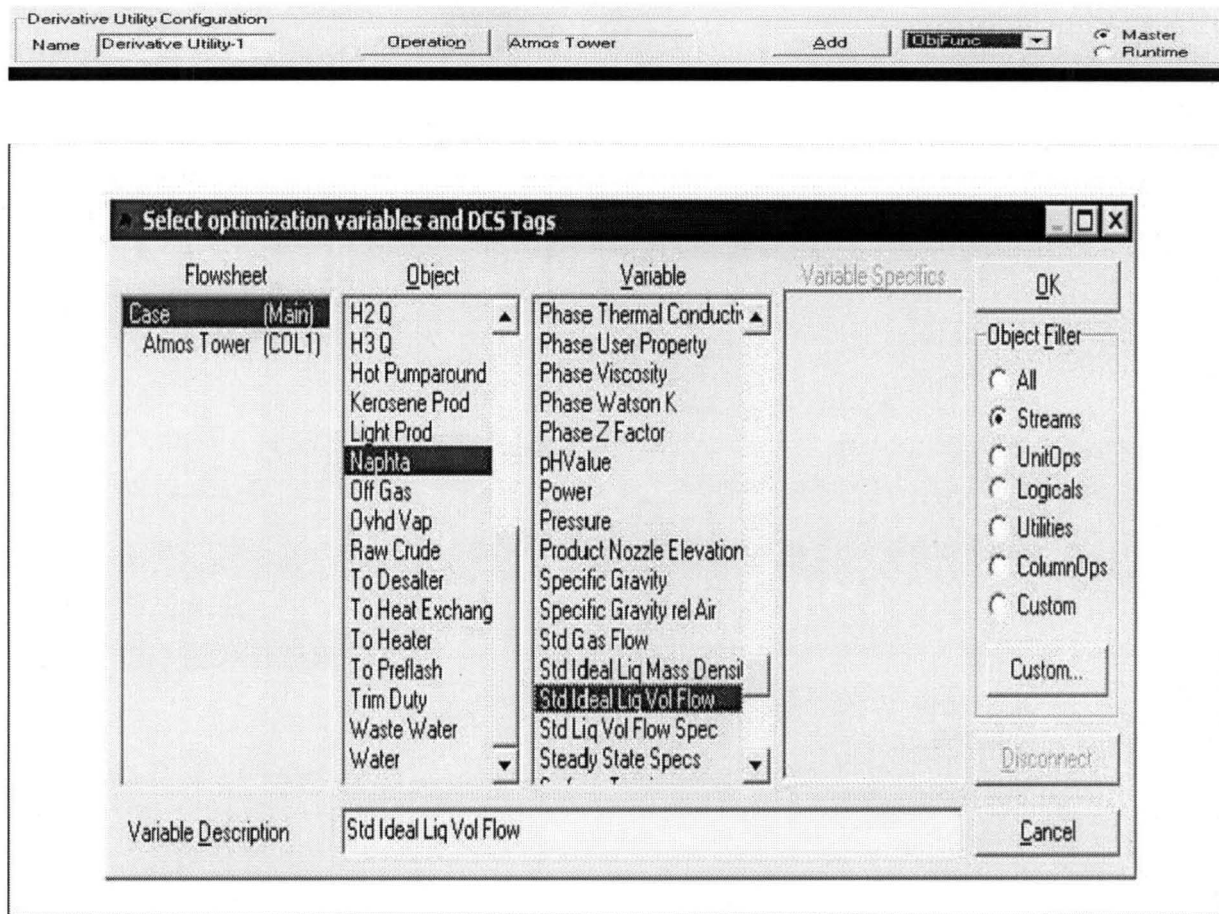


Figure 3.18 Naphta Optimization Variable Selection

33. The Configuration tab was clicked and Hyprotech SQP was selected as the optimization algorithm.
34. After all the information were configured, the Crude Distillation Unit model was run in Hysys.
35. The results were examined on the variables and constraints by opening the appropriate Derivative Utility and the Results page was viewed.

CHATER FOUR

4.0 RESULTS

The optimization, simulation and graphical results are Presented under the following headings below.

4.1 Optimization Results

The results of the optimization carried out for Base and Optimized are Presented in Tables 4.1 Below.

Table 4.1 Optimization result for base case and optimized case

Optimization Variables	Amount (m ³ /hr) Base Case	Amount (m ³ /hr) Optimized Case	Cost Per m ³ (N)	Cost Per Quantity (N) Base Case	Cost Per Quantity (N) Optimized Case
Naphtha	200.3072311	228.6293455	100,000	20,030,723.11	22,862,934.55
Kerosene	57.88960565	60.50144042	90,000	5,210,064.51	5,445,129.64
Diesel	130.3914594	135.9542195	120,000	15,646,975.13	16,314,506.34
AGO	60.86008733	71.89863288	120,000	7,303,210.48	8,627,835.95
Atm Residue	530.2721099	480.4781673	60,000	31,816,326.59	28,828,690.04
				80,007,299.82	82,079,096.51
Raw Crude	341	340.9687548	65,410	22,304,810	22,302,766.25
Heavy Crude	637.39	637.3876555	55,410	35,317,779.90	35,317,649.99
				57,622,589.90	57,620,416.24
Reboiler Duty	175900628.6	198973587.4	6.60E-06	1,160.94	1,313.23
Trim Duty	621156555.7	11762.43062	1.32E-05	8,199.27	0.155264084
				9,360.21	1313.380941
			Profit	N22,375,349.71	N24,457,543.43

4.2 Process Simulation Results

The process simulation results of Distillation Column Products are given in

Tables 4.2 through 4.7

Table 4.2 Naphtha Product Stream Properties for Base and Optimized Case

Properties	Base Case	Optimized Case
Vapour/Phase Fraction	0.0000	0.0000
Temperature: (°C)	53.13	68.40
Pressure: (kPa)	140.0	140.0
Molar Flow (kgmole/h)	1039	1754
Mass Flow (kg/h)	9.488e+004	1.747e+005
Std Ideal Liq Vol Flow (m ³ /h)	200.3	228.6
Molar Enthalpy (kJ/kgmole)	-2.014e+005	-2.133e+005
Mass Enthalpy (kJ/kg)	-2205	-2142
Molar Entropy (kJ/kgmole-°C)	50.38	47.90
Mass Entropy (kJ/kg-°C)	0.5516	0.4809
Heat Flow (kJ/h)	-2.092e+008	-3.743e+008
Molar Density (kgmole/m ³)	7.492	7.054
Mass Density (kg/m ³)	684.4	702.6
Std Ideal Liq Mass Density (kg/m ³)	731.0	764.3
Liq Mass Density @Std Cond (kg/m ³)	719.0	749.8
Molar Heat Capacity (kJ/kgmole-°C)	194.3	212.0
Mass Heat Capacity (kJ/kg-°C)	2.127	2.128
Thermal Conductivity (W/m-K)	0.1130	0.1153
Viscosity (cP)	0.3108	0.3269
Surface Tension (dyne/cm)	17.80	18.35
Molecular Weight	91.34	99.60
Z Factor	6.888e-003	6.989e-003

Table 4.3 Kerosene Product Stream Properties for Base and Optimized Case

Properties	Base Case	Optimized Case
Vapour/Phase Fraction	0.0000	0.0000
Temperature: (°C)	220.5	247.6
Pressure: (kPa)	208.6	208.6
Molar Flow (kgmole/h)	240.9	318.8
Mass Flow (kg/h)	3.493e+004	5.132e+004
Std Ideal Liq Vol Flow (m ³ /h)	57.8	60.50
Molar Enthalpy (kJ/kgmole)	-2.534e+005	-2.704e+005
Mass Enthalpy (kJ/kg)	-1748	-1680
Molar Entropy (kJ/kgmole-°C)	210.4	270.3
Mass Entropy (kJ/kg-°C)	1.451	1.679
Heat Flow (kJ/h)	-6.104e+007	-8.621e+007
Molar Density (kgmole/m ³)	4.418	4.004
Mass Density (kg/m ³)	640.5	644.6
Std Ideal Liq Mass Density (kg/m ³)	828.8	848.3
Liq Mass Density @Std Cond (kg/m ³)	805.5	826.8
Molar Heat Capacity (kJ/kgmole-°C)	395.7	449.7
Mass Heat Capacity (kJ/kg-°C)	2.729	2.793
Thermal Conductivity (W/m-K)	9.855e-002	9.817e-002
Viscosity (cP)	0.1789	0.1711
Surface Tension (dyne/cm)	10.79	10.34
Molecular Weight	145.0	161.0
Z Factor	1.150e-002	1.203e-002

Table 4.4 Diesel Product Stream Properties for Base and Optimized Case

Properties	Base Case	Optimized Case
Vapour/Phase Fraction	0.0000	0.0000
Temperature: (°C)	245.6	256.8
Pressure: (kPa)	217.1	217.1
Molar Flow (kgmole/h)	689.5	572.5
Mass Flow (kg/h)	1.436e+005	1.196e+005
Std Ideal Liq Vol Flow (m ³ /h)	130.5	136.0
Molar Enthalpy (kJ/kgmole)	-3.500e+005	-3.460e+005
Mass Enthalpy (kJ/kg)	-1681	-1656
Molar Entropy (kJ/kgmole-°C)	416.4	414.5
Mass Entropy (kJ/kg-°C)	2.000	1.984
Heat Flow (kJ/h)	-2.413e+008	-1.981e+008
Molar Density (kgmole/m ³)	3.282	3.281
Mass Density (kg/m ³)	683.4	685.6
Std Ideal Liq Mass Density (kg/m ³)	873.0	880.0
Liq Mass Density @Std Cond (kg/m ³)	847.4	857.8
Molar Heat Capacity (kJ/kgmole-°C)	567.6	572.7
Mass Heat Capacity (kJ/kg-°C)	2.726	2.740
Thermal Conductivity (W/m-K)	0.1095	0.1090
Viscosity (cP)	0.2169	0.2083
Surface Tension (dyne/cm)	13.02	12.72
Molecular Weight	208.2	209.0
Z Factor	1.534e-002	1.502e-002

Table 4.5 Atmospheric Gas Oil (AGO) Product Stream Properties for Base and Optimized Case

Properties	Base Case	Optimized Case
Vapour/Phase Fraction	0.0000	0.0000
Temperature: (°C)	279.2	306.1
Pressure: (kPa)	222.5	222.5
Molar Flow (kgmole/h)	32.72	235.5
Mass Flow (kg/h)	1.000e+004	6.575e+004
Std Ideal Liq Vol Flow (m ³ /h)	60.90	71.90
Molar Enthalpy (kJ/kgmole)	-4.849e+005	-4.233e+005
Mass Enthalpy (kJ/kg)	-1586	-1516
Molar Entropy (kJ/kgmole-°C)	756.7	696.4
Mass Entropy (kJ/kg-°C)	2.475	2.494
Heat Flow (kJ/h)	-1.586e+007	-9.966e+007
Molar Density (kgmole/m ³)	2.342	2.477
Mass Density (kg/m ³)	716.0	691.7
Std Ideal Liq Mass Density (kg/m ³)	917.4	914.4
Liq Mass Density @Std Cond (kg/m ³)	890.7	890.3
Molar Heat Capacity (kJ/kgmole-°C)	850.5	800.1
Mass Heat Capacity (kJ/kg-°C)	2.782	2.865
Thermal Conductivity (W/m-K)	0.1195	0.1097
Viscosity (cP)	0.1574	0.1228
Surface Tension (dyne/cm)	14.82	12.35
Molecular Weight	305.8	279.2
Z Factor	2.069e-002	1.865e-002

Table 4.6 Atm Residue Stream Properties for Base and Optimized Case

Properties	Base Case	Optimized Case
Vapour/Phase Fraction	0.0000	0.0000
Temperature: (°C)	344.8	353.9
Pressure: (kPa)	230.0	230.0
Molar Flow (kgmole/h)	716.8	1080
Mass Flow (kg/h)	3.028e+005	4.706e+005
Std Ideal Liq Vol Flow (m ³ /h)	530.7	480.5
Molar Enthalpy (kJ/kgmole)	-5.883e+005	-5.994e+005
Mass Enthalpy (kJ/kg)	-1393	-1376
Molar Entropy (kJ/kgmole-°C)	1303	1344
Mass Entropy (kJ/kg-°C)	3.085	3.085
Heat Flow (kJ/h)	-4.217e+008	-6.476e+008
Molar Density (kgmole/m ³)	1.722	1.693
Mass Density (kg/m ³)	727.6	737.4
Std Ideal Liq Mass Density (kg/m ³)	965.4	979.5
Liq Mass Density @Std Cond (kg/m ³)	938.7	952.1
Molar Heat Capacity (kJ/kgmole-°C)	1242	1275
Mass Heat Capacity (kJ/kg-°C)	2.940	2.926
Thermal Conductivity (W/m-K)	0.1137	0.1141
Viscosity (cP)	0.3842	0.4131
Surface Tension (dyne/cm)	12.78	12.90
Molecular Weight	422.5	435.6
Z Factor	2.599e-002	2.606e-002

4.3 Graphical Result

The graphical result obtained from the simulation and optimization is shown in

Figure 4.1

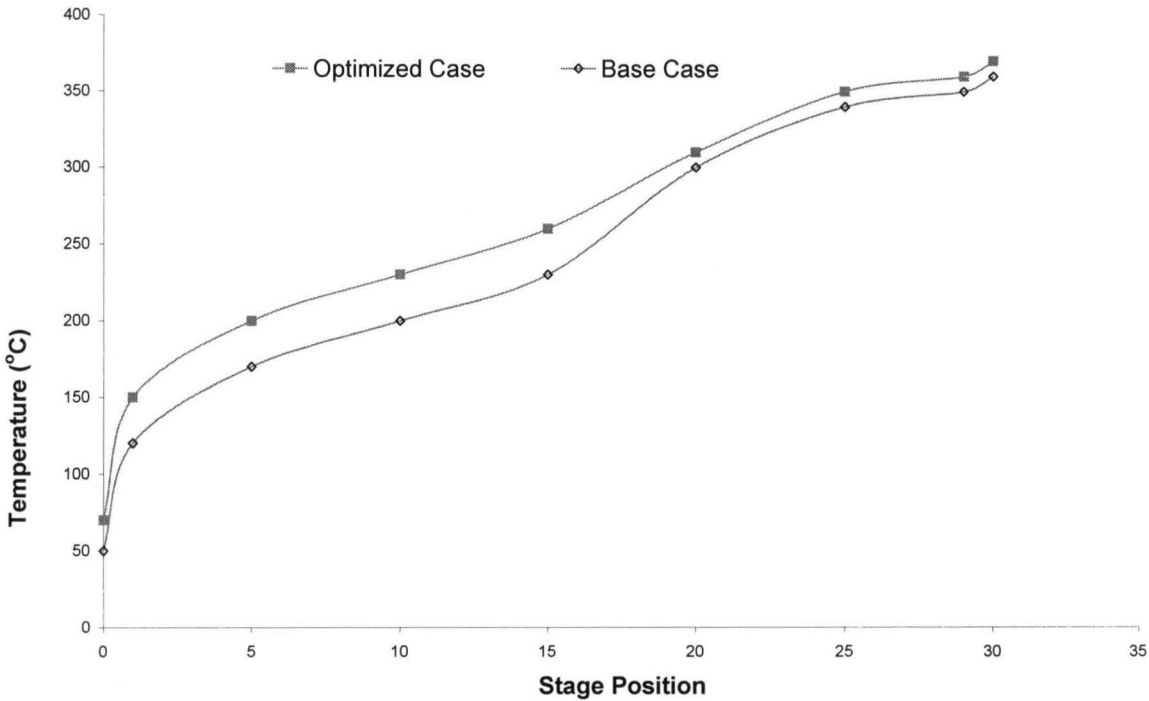


Figure 4.1 Graph of Temperature against Stage Position for the Distillation

Column for Base Case and Optimized Case

CHAPTER FIVE

5.0 DISCUSSIONS OF RESULTS

The results of the base and optimized case for the Distillation Column are discussed as follows.

5.1 Optimization Results

Table 4.1 is the results of optimization carried out for both base case and optimized case of Crude distillation Unit of Kaduna Refinery and Petrochemicals (KRPC). It showed that the cost per quantity of Naphtha obtained for both base case and optimized case are ₦20,030,723.11 and ₦22,862,934.55 respectively, and volumetric flowrate of Naphtha for both base case and optimized case are $200.3072\text{m}^3/\text{hr}$ and $228.6293\text{m}^3/\text{hr}$ respectively. This result is in agreement with the objective of this project where optimum increase in quantity of the light ends is desired. This shows that optimization of Naphtha has been carried out.

The volumetric flowrate of kerosene for both base case and optimized case are $57.8896\text{m}^3/\text{hr}$ and $60.5014\text{m}^3/\text{hr}$, while cost per quantity for both base case and optimized case are ₦5,210,064.51 and ₦5,445,129.64 respectively.

The volumetric flowrate of diesel for both base case and optimized case are $130.3914\text{m}^3/\text{hr}$ and $135.9542\text{m}^3/\text{hr}$ respectively while cost per quantity for both base case and optimized case are ₦15,646,975.13 and ₦16,314,506.34 respectively.

The volumetric flowrate of Atmospheric residue for both base case and optimized case are $530.2721\text{m}^3/\text{hr}$ and $480.4781\text{m}^3/\text{hr}$ respectively. This is because more of the residue has been converted to the lighter ends, while the cost per quantity for both the base case and optimized cases are ₦31,816,326.59 and ₦28,828,690.04 respectively.

The flowrate of Naphtha, Kerosene, Diesel and AGO are higher in the optimized case than in the base case because more of the bottom product has been converted to the lighter ends due to temperature increase. This result is in agreement with that obtained in literature (Lewin *et-al*, 1994). Literature (Chiyoda, 1973) also states that decreasing the quantity of the bottom product (atmospheric residue) increases the quantity of the other lighter ends. The result is also in agreement with the objective of this project which is to increase quantity of the lighter ends which generates more revenue and reduce the quantity of the bottom product which is cheaper. This is the essence of the optimization.

The quantity of Raw Crude and Heavy Crude for both the base case and optimized case remain the same, equal values of Raw materials was also used for base case and optimized case by (Lewin *et-al*, 1994) in order to see the effect of the optimization carried out.

Fundamental of optimization also suggests that raw materials values should be constant for both base case and optimized case in an optimization problem. (Lewin *et-al*, 1994) and Chiyoda (1980).

Profit realized from both base case and optimized cases are ₦22,375,349.71 and ₦24,457,543.43 respectively. The result showed that the objective of the optimization of the Crude Distillation Unit I (CDU I) to increase profitability is achieved.

5.2 Simulation Results

Tables 4.2 through 4.6 showed that Naphtha, Kerosene, Diesel and AGO Product volume flowrate increased appreciably from 200.3m³/hr to 228.6m³/hr, 57.883m³/hr to 60.503m³/hr, 130.393m³/hr to 135.953m³/hr and 60.863m³/hr to 71.893m³/hr respectively from base to optimized case, with a corresponding temperature increase from 53.13°C to 68.40°C, 220.5°C to 247.6 °C, 245.6 °C to 256.8 °C and 279.2 °C to 306.1°C respectively. The increase in temperature is as a result of increase in heat supply by reboiler in heating up the crude to increase the lighter ends. This result is also in total agreement with literature (Lewin et-al, 1994) where increase in reboiler duty of Crude Distillation Unit increased the quantity of the lighter ends obtained from the unit.

Table 4.6 showed that Atmospheric residue Product volume flowrate decreased appreciably from 530.7m³/hr to 480.53m³/hr due to conversion into the lighter ends from base to optimized case, and the temperature increased from 344.8 °C to 353.9 °C as a result of increase in the reboiler duty. The result is also in agreement with the objective of this project because the optimization requires increase in quantity of the lighter ends which generates more revenue and reduction in the quantity of the bottom product which is cheaper.

5.3 Graphical Result

Figure 4.1 presented in Chapter Four is the Graphical result obtained from the process simulation and optimization and is discussed below.

5.3.1 Temperature comparison of base case and optimized case for the distillation column

The plot of Figure 4.1 shows that the base case condenser temperature is 50°C while that of the optimized case is 60°C. The plot also showed that the base case temperature increased from 50°C to 170°C from condenser stage to tray 5 while that of the optimized case increased from 60°C to 200°C. The plot also showed that the temperature increased from 170°C to 350°C for the base case, while that of the optimized case increased from 200°C to 360°C from stage 5 to the last stage (i.e. tray 29) respectively. Lewin *et-al*, (1994) stated that increase in temperature is as a result of increase in reboiler duty.

CHAPTER SIX

6.0 CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusions

The following conclusions may be drawn from the results of the analysis.

1. Optimization was carried on Crude Distillation Unit I (CDU I) of Kaduna Refinery and Petrochemicals (KRPC)
2. The volumetric flowrates of Naphtha, Kerosene, Diesel and AGO are higher in the optimized case than in the base case, while that of the Atmospheric residue decreased after the optimization due to conversion..
3. The optimization carried out showed that the Plants profit rose from N22,375,349.71 to N24,457,543.43.

6.2 Recommendations

Based on the analysis carried out the following are recommended:

1. The Nigerian National Petroleum Corporation should carry out optimization for the other fractions (Kerosene, Diesel and AGO) of Crude Distillation Column of KRPC.
2. The Nigerian National Petroleum Corporation should carry out optimization for the other units of KRPC Plant.

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