	Million
GEORGIA INSTITUTE OF TECHNOLOGY	OFFICE OF CONTRACT ADMINISTRATION
	x ORIGINAL
PROJECT ADMINISTRATION	DATA SHEET REVISION NO.
Project No	DATE: 8/17/81
Project Director: Dr. William J. Wepfer	School/MMX Mechanical Engineering
Sponsor: United Engineering Trustees, Inc., Engi	neering Foundation
Type Agreement: Grant No. RC-A-80-1C	(m. c) (1/02 (m. c))
Award Period: From <u>9/1/81</u> To <u>9/1/82</u>	(Performance) 9/1/82 (Reports)
Cost Sharing: $$6.510 (F-25-352)$	Contracted through:
Title: Thermo-Economic Analysis, Design and Or	timization of Energy Systems
ADMINISTRATIVE DATA OCA CC	NTACT Faith G. Costello
1) Sponsor Technical Contact: -See Below-	
2) Sponsor Admin./Contractual Contact: Mr. John	A. Zecca, Secretary and General Manager,
United Engineering Trustees, Inc., Engineering	Soc. Lib., Engineering Foundation,
United Engr. Ctr., 345 East 147th St., New Yor	:k, NY 10017
Reports: See Deliverable Schedule Security Cl	assification: N/A
Defense Priority Rating: N/A	
DECENTIONS	n far en fan in de fan it de fan it de fan it de fan de fan it de fan i I
<u>RESTRICTIONS</u>	for the Chart for Diditional Deguinement
See Attached N/A Supplemental I	nformation Sheet for Additional Requirement
travel requires sponsor approval where t 125% of approved proposal budget categor	- Contact OCA in each case. Domestic otal will exceed greater of \$500 or Y.
Equipment: Title vests with Sponsor; however,	none proposed.
	10° A 003
COMMENTS:	
	RECEIVED
	Research Reports
	Unice
COPIES TO:	217151
Administrative Coordinator Research Securit	y Services EES Research Public Relations
Research Property Management . Reports Coordina	tor (CCA) Project File (OCA)
Procurement/FES Supply Services tileary madui	OLAJ Other:

#### GEORGIA INSTITUTE OF TECHNOLOGY

OFFICE OF CONTRACT ADMINISTRATION

#### SPONSORED PROJECT TERMINATION SHEET

#### Date 9/22/82

Project Title: Thermo-Economic Analysis, Design and Optimization of Energy Systems

Project No: E-25-646

Project Director: Dr. William J. Wepfer

Sponsor: The Engineering Foundation

Effective Termination Date: 9/1/82

Clearance of Accounting Charges: 9/1/82

Grant/Contract Closeout Actions Remaining:

Final Invoice and Closing Documents

**Final Fiscal Report** 

**Final Report of Inventions** 

Govt. Property Inventory & Related Certificate

**Classified Material Certificate** 

Other \_\_\_\_\_

Assigned to: \_\_\_\_\_ Mechanical Engineering (School/Laboratory)

#### COPIES TO:

Administrative Coordinator Research Property Management Accounting Procurement/EES Supply Services

Research Security Services **Reports Coordinator (OCA)** Legal Services (OCA) Library

**EES Public Relations (2) Computer Input Project File** Other

**FINAL REPORT** 

E-25-646

# THERMO-ECONOMIC ANALYIS, DESIGN, AND OPTIMIZATION OF ENERGY SYSTEMS

# BY

William J. Wepfer Assistant Professor and Principal Investigator

H. A. Cikanek III
R. M. Garceau
B. B. Moore
Graduate Research Assistants

**Prepared** for

The Engineering Foundation United Engineering Trustees, Inc. Grant No. RC-A-80-IC

# 31 August 1982

# **GEORGIA INSTITUTE OF TECHNOLOGY**

A UNIT OF THE UNIVERSITY SYSTEM OF GEORGIA SCHOOL OF MECHANICAL ENGINEERING ATLANTA, GEORGIA 30332



#### THERMOECONOMIC ANALYSIS DESIGN AND

#### OPTIMIZATION OF ENERGY SYSTEMS

#### Final Report

By

William J. Wepfer Assistant Professor and Principal Investigator

Harry A. Cikanek III Robert M. Barceau Bryan B. Moore Graduate Research Assistants

#### School of Mechanical Engineering Georgia Institute of Technology Atlanta, GA 30332

August 31, 1982

## Prepared for

The Engineering Foundation United Engineering Trustees, Inc. Grant No. RC-A-80-1C

William J. Wepfer, Principal Investigator

Brighton, Director John//A. School of Mechanical Engineering

#### ACKNOWLEDGEMENTS

The work presented in this report was carried out with the support of the Engineering Foundation Grant RC-A-80-1C. Additional support was provided by the Georgia Institute of Technology, the Gulf Oil Foundation (one graduate fellowship), and Celanese Corporation (one graduate fellowship). Any findings, conclusions, and recommendations expressed here are those of the authors and do not necessarily reflect the views of the Engineering Foundation, Georgia Tech, Gulf Oil Foundation, and Celanese Corporation.

#### ABSTRACT

The primary goal of this project was the development and advancement of thermoeconomic methods applied to the improvement of design concepts as well as the economic optimization of process designs. This goal has been met in large part with the development of design methodologies for use with separation systems and cogeneration.

However, a major disappointment involved the lack of progress toward the development of a Second Law based simulation program, due to difficulties encountered in obtaining the appropriate software on which to build. At this writing, the authors have debugged and revised SOLTES (Simulator of Large Thermal Systems, developed at Sandia Laboratories) for use on the Georgia Tech computer. SOLTES is now ready to be modified for use as a Second Law based analysis and simulation program (Chapter One).

The development of a design methodology for application to separation processes (Chapter Two) required the derivation of an expression for the entropy production due to the mass fluxes in binary mass transfer systems. The entropy production was then transformed into a function of the process variables including reflux ratio (column height) and inlet and exit mole fractions. The optimal design strategy

iii

required the application of a money balance to each system component - reboiler, condenser, and tower - for the purpose of obtaining intercomponent unit costs. In turn these costs along with an initial set of design variables, capital costing equations as functions of the design variables, and the unit costs of utilities, were used to optimize the column, reboiler, and condenser. This procedure was repeated until the design variables and unit costs converged -- typically in two iterations.

The results of applying this procedure to a simple system compared very favorably with traditional methods. The primary advantage of this Second Law methodology is the fact that the optimization of a complex separation system is greatly simplified by breaking the system into its individual components for subsequent suboptimization.

A new method for the optimal design of a simple cogeneration system was developed. This approach, which incorporates LaGrange's method, represents a modification and extension of previous work by Evans (42) and El-Sayed and Tribus (31). This application required the development of costing equations as functions of the decision variables via an extensive literature search as well as communications with vendors. In a departure from previous work, the requirement that the decision variables must have an associated available energy flow was relaxed entirely. Use of steam table data required the introduction of numerical methods for the evaluation of the marginal and shadow price vectors.

iv

This technique assumes an initial working design which need not be close to optimum. The shadow price vector is evaluated and used to generate the marginal price vector. A new set of decision variables is then selected based on the signs and magnitudes of each entry of the marginal price vector. This process is repeated until the magnitude of the marginal price vector attains a predetermined small stable value.

In addition, this approach was used to suboptimize the system at various fixed electrical outputs. As a consequence these suboptimizations will be only functions of the price of electricity, and will depend only on the relative costs of fuel, equipment, and capital. Then, given a market or regulated price for electricity, the best overall design can be selected from the suboptimizations. As a demonstration of this technique, net revenue curves were generated as functions of work/heat ratio for various fuel costs and market prices of electricity.

# TABLE OF CONTENTS

ACK	NOWLE	DGEMENTS					•	• •	•						•	]	Page ii
ABS	TRACT				• •							1.				.i	lii
LIS	TOF	FIGURES															ix
LIS	T OF '	TABLES.				•						į.					xi
1.	DEVE LAW	LOPMENT ( ANALYSIS	OF A CO AND SI	MPUTE	ER PI	ROGI	RAM	FO	R 5	SEC	CON	ID					1
	1.1	Introdu	ction .			• •	•						•			•	1
	1.2	Construe	ction o	f Sys	stem	Log	gic		•				•				1
	1.3	Property	y Compu	tatio	on.			•	•								5
		1.3.1.	SOLTES	Prop	perty	7 Co	ompu	ıta	tid	ons	з.		•				5
		1.3.2.	Proper	ty Co	omput	ati	lons	s f	or	St	ea	m.	•				6
		1.3.3.	Proper Real G	ty Co ases	omput	ati	lon	fo	r : •	[de	eal	- 8	an	d			7
	1.4	Simulat	ion and	Effi	lcier	ncy	Ana	aly	si	5.			•	•	•		8
	1.5	Costing	of Flor	w Sti	ceams	s	•		•				•	•	•		9
	1.6	Optimal	Design			•			•								9
	1.7	Conclus	ions and	d Red	comme	enda	atic	ons									10
2.	APPL: OPTI	ICATION ( MIZATION	OF SECO TO MAS	ND LA S TRA	AW BA ANSFI	ASEI ER I	D DE PROC	ESI CES	GN SE S	5.			•		•		12
	2.1	Introduc	ction .				•						•				12
	2.2	Derivat: Equation	ion of	the H	Entro	ру	Pro	odu •	ct:	Lor	1		•			•	13
		2.2.1.	Flow C	onfig	gurat	ior	ı.	·		• •			•	•	•	•	13
		2.2.2.	Thermo	dynan	nic (	Gove	erni	ing	E	qua	ati	or	ns	•	•	•	13

	2.3	Application to Simple Tower Design 19
		2.3.1. System Description
		2.3.2. Available-Energy Analysis
		2.3.3. Thermoeconomic Governing Equations 23
		2.3.4. Optimization Procedure
	2.4	Results and Conclusions
	2.5	Closure
3.	COGE SYST	NERATION AND THE LAGRANGE METHOD OF EM OPTIMIZATION
	3.1	Cogeneration
	3.2	Optimization Procedure Using Lagrange's Method
	3.3	Closure
4.	OPTI SYST	MIZATION OF A RANKINE CYCLE COGENERATION EM
	4.1	Introduction
	4.2	Objective Function
	4.3	Cost Estimation
		4.3.1. Boiler Costing Equation 52
		4.3.2. Turbine-Generator Costing Equations 57
		4.3.3. Condenser Costing Equations 60
		4.3.4. Pump Costing Equations 64
		4.3.5. Fixed Charges
	4.4	Optimization Procedure 67
5.	RESU	LTS OF COGENERATION OPTIMIZATION 82
	5.1	Computer Program Operation and Application 82
	5.2	Results of Suboptimizations 85
	5.3	Comparison with Alternative and the Selection of Overall Optimum

5.4 Rece	ommendation Concerning the Optimiza-	
tion	n of a Cogeneration System	96
6. REVIEW O	F BUDGET	.04
7. PUBLICAT	IONS AND PRESENTATIONS 1	.06
APPENDICES .		.07
APPENDIX A.	COMPUTER PROGRAMS GETZ AND LOOKUP FOR THERMODYNAMIC PROPERTY EVALUATION 1	.08
APPENDIX B.	COMPUTER CODES FOR OPTIMAL DESIGN OF A BINARY SEPARATION SYSTEM 1	.14
APPENDIX C.	THE LAGRANGE METHOD OF UNDETERMINED MULTIPLIERS	.42
APPENDIX D.	LAGRANGE'S METHOD USING JACOBIANS 1	.45
APPENDIX E.	DERIVATION OF SHADOW AND MARGINAL PRICE EQUATIONS	.50
APPENDIX F.	COMPUTER PROGRAM USED TO OPTIMIZE THE COGENERATION SYSTEM	.61
APPENDIX G.	OPTIMAL DESIGN DATA FOR THE COGENERATION SYSTEM	.87
REFERENCES .		.00

# LIST OF FIGURES

.

]	Figure		]	Page
	2.1.	Schematic Diagram Showing the Model of the Two Phase Binary Mass Transfer System		14
	2.2.	Schematic Diagram of the Binary Distillation System		20
	3.1.	Available Energy and (Energy) Analysis for an Industrial Rankine Cycle Cogeneration System		34
	3.2.	Graphical Interpretation of a Negative Marginal Price	•	44
	3.3.	Graphical Interpretation of a Positive Marginal Price	•	44
	4.1.	Rankine Cycle Cogeneration System		49
	4.2.	Base Boiler Cost Versus Steam Mass Flow Rate	•	54
	4.3.	Boiler Pressure Drop Factor Versus Boiler Pressure Drop Coefficient	•	55
	4.4	Boiler Efficiency Factor Versus Boiler Efficiency	•	55
	4.5	Boiler Temperature Factor Versus Temperature	•	56
	4.6.	Turbine Isentropic Efficiency Factor Versus Turbine Isentropic Efficiency	•	59
	4.7	Turbine Temperature Factor Versus Temperature .		59
	4.8.	Shell and Tube Side Pressure Loss Factors Versus Pressure Loss	•	61
	4.9.	Condenser Pressure Factor Versus Condenser Pressure	•	63
	4.10.	Condenser Temperature Factor Versus Minimum Temperature Difference		63

4.11.	Pump Base Cost Versus Pump Work	65
4.12.	Pump Isentropic Efficiency Factor Versus Pump Isentropic Efficiency	65
4.13.	Steam Cycle for the Cogeneration System in T-S Coordinates	68
5.1.	Optimum Boiler Efficiency Versus Work/Heat Ratio	86
5.2.	Optimum Pump Efficiency Versus Work/Heat Ratio	86
5.3.	Optimum Condenser Inlet Pressure Versus Work/Heat Ratio	90
5.4.	Optimum Turbine Inlet Pressure Versus Work/Heat Ratio	90
5.5.	Optimum Boiler Pressure Drop Coefficient Versus Work/Heat Ratio	92
5.6.	System Second Law Efficiency Versus Work/Heat Ratio	92
5.7.	Equipment Cost Versus Work/Heat Ratio	93
5.8.	Net Revenue Generated Versus Work/Heat Ratio for a Fuel Cost of \$2/10 <sup>6</sup> Btu	97
5.9.	Net Revenue Generated Versus Work/Heat Ratio for a Fuel Cost of \$3/10 <sup>6</sup> Btu	98
5.10.	Net Revenue Generated Versus Work/Heat Ratio for a Fuel Cost of \$4/10 <sup>6</sup> /Btu	99

# LIST OF TABLES

Table			Page
2.1.	System Design Information		21
2.2.	Available-Energy Balance Equations	•	22
2.3.	Results of Second Law Optimization	•	30
4.1.	Amortized Costing Equations for the Cogeneration System		66
4.2.	Equations of Constraint for the Cogeneration System	•	69
4.3.	Fixed Parameters and Decision Variables for the Cogeneration System		70
4.4.	Shadow Price Matrix for the Cogeneration System		76
4.5.	Shadow Price Equations for the Cogeneration System	•	77
4.6.	Marginal Price Matrix for the Cogeneration System	•	78
4.7.	Marginal Price Equations for the Cogeneration System	•	80
5.1.	Parametrically Varied Fixed Variables for the Cogeneration System		84
6.1.	Budget Review	•	105
G.1.	Optimal Decision Variables	•	188
G.2.	Selected Optimized State Variables		191
G.3.	Optimized Capital Investments, Fuel Input, and Second Law Efficiency		194
G.4.	Net Revenue Generated on a Sale of Electricity		198

xi

# 1. DEVELOPMENT OF A COMPUTER PROGRAM FOR SECOND LAW ANALYSIS AND SIMULATION

## 1.1 Introduction

The original goal of this project, the development of a complete software package for Second Law analysis and simulation of thermal systems, could not be fully realized, principally because of difficulties in obtaining the appropriate software on which to build. Such a program, entitled SOLTES, was obtained six months into the project. In the meantime, work was invested in the development of optimal design strategies, with application to separations systems and cogeneration.

#### 1.2 Construction of System Logic

The primary goal of Part I of this work was the construction of program logic for a modular analysis and simulation code. It was originally hoped that this logic would be patterned after logic found in one of the well-known simulation programs. However, difficulties arose: ASPEN, a DOE-funded generalized simulation program, is still not available to the general public (it was to have been available in Fall 1981). TRNSYS (1), a well-known solar simulation program, was found to be unacceptable. General Electric's THERMS (2) program was found to be too simple. In late February 1982 a program entitled SOLTES-1B was received from the National Energy Software Center at Argonne Laboratories, which satisfied all criteria for the purposes of this grant.

SOLTES (Simulator of Large Thermal Energy Systems) simulates the steady state response of thermal/power systems to time varying load and weather data. Thermal energy system models can be modularly constructed from a library of routines that includes pumps, boilers, heat exchangers, extraction turbine-generators, condensers, regenerative heaters, and process heating loads, as well as user-supplied routines. A load management routine allows SOLTES to simulate total energy/ cogeneration systems that follow process heat or power loads and demands.

SOLTES was received at Georgia Tech in the form of a tape having 53 separate files, a transmittal memo, and a 300-page user's manual. The SOLTES code was written in FORTRAN IV for use on a CDC 6600 mainframe computer at Sandia Laboratories. SOLTES consists of a preprocessor that creates input files on an interactive basis, a partial main simulation program that is completed by the preprocessor, and a large user library (145 subprograms).

The SOLTES tape includes source files for the user library, machine-specific block data transfer subroutines, the preprocessor PRESOL, and the partial main program. Input data files necessary to run two example problems and a file of weather data for Albuquerque, N.M., were also included on the tape.

The user's manual (3) and the transmittal memo contained some of the background information necessary to run SOLTES. However, this background material was not complete.

Activating this software required a number of tasks which began with reading the tape into mass storage in an account on the Georgia Tech CDC Cyber 170-760/170-730. Each of the files was stored and listings were printed for later use.

Running the example problems was the next task to be tackled. Example #1 involved the simulation of a residential solar hot water system having 11 components and timevarying weather data. To complete this problem it was first necessary to use PRESOL to create the input files for the main program. Incomplete documentation led to lengthy phone conversations with SLA (Sandia Laboratory) personnel to learn exactly how the preprocessor worked. It appeared that the preprocessor could be run in the batch mode using files from the tape to drive it. However, that effort failed. Thus the preprocessor was run in the interactive mode using data stored in files. During a PRESOL run, the main program was also created (really completed) and saved. These newly constructed input files and mainline were then successfully executed to complete Example #1.

Example #2 consisted of a Rankine-solar total energy system having 25 components and a time-sharing load data capability. This example was to be run in the batch mode

since the main program and all of its input files were already created and contained on the tape. Most of the transmittal memo control statements for the SLA CDC 6600 were compatible with the Georgia Tech CDC machine. However, the documentation did not explain the operation of the control statements so that many hours were spent in order to convert the few incompatible control statements into usable form.

Inadequate documentation led to another problem. Each of the modular components has an associated set of constants that must be stored and used in the next time step. These are stored outside of core memory by way of machine-dependent extended core storage (ECS) subroutines written in CDC assembly language. To finally run the two example problems, ECS capability had to be initiated, and the two machine dependent ECS routines (SLA and Georgia Tech) had to be merged into a user library.

Unfortunately, Georgia Tech will be discontinuing its ECS capability. An alternative strategy for storing the large array of data was implemented through the use of virtual memory subroutines. New subroutines are currently being written to run the virtual memory routines without altering any of the non-machine dependent software but at the cost of many working hours.

Concurrently, as a final test of system logic and compatibility, a Rankine cycle cogeneration system was devised and simulated. At this point in time the SOLTES

program provides a good working framework and system logic for the inclusion of Second Law analysis postprocessor routines, as well as economic analysis postprocessors.

## 1.3 Property Computation

A primary goal of this project was the development of subroutines for the evaluation of the property, available energy. Some work was initiated before the SOLTES program was obtained, and still needs to be integrated into the Georgia Tech version of SOLTES system library.

## 1.3.1 SOLTES Property Computations (3)

Component routines that model components in Rankinetype power cycles require only constants to characterize the working fluid. These constants and the properties of heat-transfer fluids, as functions of temperature, are stored and retrieved from a fluid property data file by fluid name. Thus only the fluid name is required as SOLTES input, provided the fluid property data for the fluids in the system model exist in the fluid property data bank.

Fluid property data files contain the constants used to compute heat-transfer fluid properties as a function of temperature, as well as the constants that characterize power-cycle working fluids. Calculations of the heattransfer fluid properties -- density, heat capacity, thermal conductivity, and viscosity -- are based on polynomial fits

of measured data, over two ranges of temperature (a hightemperature range and a low-temperature range).

The constants that characterize each power-cycle fluid include: molecular weight, normal boiling point, critical temperature, critical volume, the acentric factor, reference liquid density, reference temperature for the liquid density, four constants for use in an ideal gas heat capacity equation, heat of vaporization at the normal boiling point, and Goldhammer's constant.

At this writing it appears that the SOLTES code can be easily adjusted for inclusion of available energy computations. This is because sufficient information already exists for the computation of enthalpy, entropy, and free energy -- each of which is necessary for available energy evaluations. If not, the following work which was performed prior to receiving SOLTES can be integrated into SOLTES.

# 1.3.2 Property Computations for Steam

Because Rankine cycle systems are so common (central station power plants, total energy, cogeneration), it is desirable to include explicit evaluation of steam table property data. This can be accomplished via the subroutine STEAM (4). Plans do exist for the modification of SOLTES to include an option whereby STEAM will be used to evaluate power-cycle and heat-transfer properties.

#### 1.3.3 Property Computation for Ideal and Real Gases

Early in the project the program GASES was obtained (5, 6). This program does a complete Second Law analysis of a unit process having only inflows and outflows of materials that behave as ideal gases. It was hoped that this program could be extended to include flows of materials that behave as real gases.

It was decided that the best approach for computing real gas corrections was by way of calculation of the compressibility factor and enthalpy and entropy deviations as functions of reduced temperature, reduced pressure, and acentric factor (7, 8). Furthermore, a decision was made to utilize a set of tabular data from Lewis and Randall (7) for evaluation of the compressibility, enthalpy deviation, and entropy deviation. The complete set of subroutines, programs, and data files for this task consists of two subroutines, twelve data files, and three utility routines.

Subroutine GETZ returns a value of z, the compressibility factor, given inputs of reduced pressure, reduced temperature, and the acentric factor. GETZ determines whether the input values of reduced temperature and pressure are in the proper range and which tabular data to use: that for gases (the main tables), the tables for data near the two-phase region, or the tables for data near the critical region. If the input data isn't in the proper range, a value of zero is returned for z.

GETZ operates by first opening the file for the appropriate table. Then given reduced temperature and pressure the subroutine LOOKUP finds the corresponding value of  $z^{(0)}$  and/or  $z^{(1)}$  (where  $z = z^{(0)} + wz^{(1)}$  with w as the acentric factor (7)) from one of six files which contain the tabular data.

The subroutines GETZ and LOOKUP can also be used to obtain values for enthalpy deviation and entropy deviation. The only additional items that are needed include the data files which contain the raw data (Tables A1-10 - A1-15 in Reference 7). This will be undertaken at a later time. Appendix A contains printouts of GETZ and LOOKUP.

At some point this scheme will need to be tested against the property evaluation scheme already contained in SOLTES. A decision will then need to be made regarding which approach should be pursued.

#### 1.4 Simulation and Efficiency Analysis

The SOLTES code includes virtually all of the necessary modular components including boilers, condensers, cooling towers, heat exchangers, load management, mixers, make-up water sources, pipes, process heat and vapor loads, pumps, regenerative heaters, four different turbine models, flow dividers and throttling valves. In addition SOLTES contains two system performance routines: energy accounting and energy summing.

Because of the aforementioned difficulties, no progress has yet been made to include Second Law efficiency analysis. However, now that the SOLTES program has been debugged for use on the Georgia Tech computer, two tasks need to be performed. First, each of the modular components need to be modified to include the computation and output of available energy consumption and Second Law efficiency. This is an almost trivial task if given proper available energy property computation routines (see Section 1.3). Second, the energy accounting and summing routines need to be copied for available energy accounting and summing. Again, this is an easy task.

## 1.5 Costing of Flow Streams

Because of the aforementioned difficulties no progress has been made to include any kind of economic analysis or flowstream costing schemes. It is anticipated that a postprocessor that incorporates such economic analyses will be written at a later time.

# 1.6 Optimal Design

Significant progress was made in this area. Because of the difficulties in finding and obtaining the SOLTES code, and because of commitments to graduate students, it was decided that substantial effort would be exerted in this area. Chapter 2 contains a complete description of the work performed on the application of Second Law design

methodology to separation systems. Chapters 3-5 describe the application of a design methodology to a Rankine cycle cogeneration system. In both these applications, computer software was developed which can be used in conjunction with SOLTES for optimal design as well as integrated performance analysis over the operating life of the system.

## 1.7 Conclusions and Recommendations

At this point in time SOLTES provides an excellent tool that can be extended to include the various requisites for Second Law and economic analyses. It is the intention of the principal investigator to complete the following tasks:

- 1. Inclusion of steam table property data.
- Development of available energy property computation techniques.
- 3. A sensitivity study to determine which of the two current techniques (method in SOLTES, or the use of Pitzer's tabular data) for computing real gas properties is better.
- Modification of the modular subroutines to include the computation of available energy consumption and Second Law efficiency.
- Duplication of the energy accounting and summing postprocessors for conversion into available energy accounting and summing postprocessors.

 Development of a compatible economic postprocessor.

The principal investigator currently has proposals pending for support of this work.

#### 2. APPLICATION OF SECOND LAW BASED DESIGN OPTIMIZATION TO MASS TRANSFER PROCESSES

2.1 Introduction

In general Thermoeconomic Optimization requires the derivation of expressions for entropy production, via nonequilibrium thermodynamics, due to each independent extensive property transport. In order to obtain such expressions, it is necessary to apply thermodynamic property relations for multi-component systems in conjunction with material and energy balances, heat, mass, and momentum transport equations.

Once the necessary expressions for the entropy productions are developed, the thermodynamic variables must be transformed into the relevant process design variables. These various equations can then be coupled with capital cost expressions to allow system optimization by any current technique (Lagrange multipliers, Surrogate worth trade-off, ...).

Specifically this chapter describes an expression for the entropy production due to the mass fluxes in binary masstransfer systems with application to continuous differential contactors. A stagnant film model is used for two-phase boundaries (11, 12), which in effect, isolates the mass transfer process to a thin region at the interface stagnant film. Once the expressions for entropy production in terms of pressure, temperature, and composition are available a transformation is made to process variables such as reflux ratio, column height, packing or tray geometry, column diameter and column efficiency.

Results of this design optimization model are compared with the results obtained via traditional methods.

# 2.2 Derivation of the Entropy Production Equation

# 2.2.1 Flow Configuration

Consider a two-phase, binary mass transfer system as shown in Figure 2.1. It is assumed that a stagnant film region exists such that 1) the vapor and liquid are in equilibrium, 2) there is a net transfer of component A from liquid to vapor and a corresponding net transfer of component B from vapor to liquid, and 3) the bulk flow of vapor and liquid in the z-direction within the stagnant film is negligible. As the derivation proceeds, the constant molal overflow assumption will be invoked (12). In addition, a form of the Gibbs equation will be used to eliminate the time derivatives. Finally, heat transfer effects within the column will be neglected. The resulting expression for steady state entropy production arising from mass transfer in a binary system will be cast in terms of the process variables.

#### 2.2.2 Thermodynamic Governing Equations

Derivation of the expression for entropy production arising from mass transfer requires application of the fundamental balance equations. Initially potential and kinetic energy as well as momentum effects are neglected. With these assumptions the governing equations are given as follows:

Mass

$$\frac{\partial \rho_{i}}{\partial t} + \nabla \cdot \underline{\dot{n}}_{i} = 0$$
 (2.1)



Figure 2.1. Schematic diagram showing the model of the two phase binary mass transfer system.

15

Energy

 $\frac{\partial(\rho u)}{\partial t} + \nabla \cdot \underline{u} = 0$  (2.2)

Entropy

$$\frac{\partial(\rho s)}{\partial t} + \nabla \cdot \underline{s} = \dot{s}_{p}$$
(2.3)

Entropy Current Density (13,14)

$$\frac{\dot{s}}{\underline{s}} = \frac{1}{\underline{T}\underline{u}} + \sum \frac{\mu_{\underline{i}}}{\underline{T}\underline{n}\underline{i}}$$
(2.4)

Time Derivative of the Gibbs Equation (13, 14)

$$\frac{\partial(\rho u)}{\partial t} = T \frac{\partial(\rho s)}{\partial t} + \sum \mu_{i} \frac{\partial \rho_{i}}{\partial t}$$
(2.5)

Taking the divergence of Eq. 2.4 and solving for  $T(\nabla \cdot \dot{s})$  yields

$$T(\nabla \cdot \underline{\dot{s}}) = \nabla \cdot \underline{\dot{u}} - \underline{\dot{s}} \cdot \nabla T - \sum \mu_{i} (\nabla \cdot \underline{\dot{n}}_{i}) - \sum \underline{\dot{n}}_{i} \cdot \nabla \mu_{i}$$
(2.6)

Substitution of Eq. 2.6 into the entropy balance yields

$$T\frac{\partial(\rho s)}{\partial t} = \sum \mu_{i}(\nabla \cdot \underline{\dot{n}}_{i}) + \sum \underline{\dot{n}}_{i} \cdot \nabla \mu_{i} + \underline{\dot{s}} \cdot \nabla T - \nabla \cdot \underline{\dot{u}} + T\dot{s}_{p} \qquad (2.7)$$

Eq. 2.7 can be further simplified by substitution of the mass and energy balance equations

$$T\frac{\partial(\rho s)}{\partial t} = -\sum_{\mu} \frac{\partial^{\rho} i}{\partial t} + \frac{\partial(\rho u)}{\partial t} + \frac{i}{s} \cdot \nabla T + \sum_{\mu} \frac{\dot{n}}{i} \cdot \nabla \mu_{i} + T\dot{s}_{p} \qquad (2.8)$$

However, a form of the Gibbs Equation, Eq. 2.5, can be factored out of Eq. 2.8 to give

$$T\dot{s}_{p} = -\underline{s} \cdot \nabla T - \sum \dot{\underline{n}}_{i} \cdot \nabla \mu_{i}$$
(2.9)

Equation 2.9 relates the basic extensive properties, the respective driving potentials, and the entropy production in the diffusion process. The first term,  $s \cdot \nabla T$ , arises from heat

transfer effects while the second term is due to mass transfer. If the effects of column heat transfer are neglected, Eq. 2.9 simplifies to

$$T\dot{s}_{p} = -\sum_{\underline{n}} \dot{\underline{n}}_{i} \cdot \nabla \mu_{i}$$
(2.10)

Employing the geometry of Figure 1, Eq. 2.10 is reduced to a one-dimensional form

$$Ts_{p} = -n_{A}\frac{d\mu_{A}}{dx} - n_{B}\frac{d\mu_{B}}{dx}$$
(2.11)

To obtain the total entropy production in the tower, Eq. 2.11 must be integrated over the total diffusion volume

$$\int_{V} T\dot{s}_{p} dV = \int_{V} \left[ -n_{A} \frac{d\mu_{A}}{dx} - n_{B} \frac{d\mu_{B}}{dx} \right] dV \qquad (2.12)$$

The volume differential, dV, can be expressed in terms of cartesian coordinates dxdydz. The mass flux normal to the interface is a function of the concentration difference between the bulk fluid and the interface (at which the liquid and vapor are in equilibrium) which is a function of tower height, z, in the column. Integration of Eq. 2.12 over dxdydz yields

$$-TS_{p} = \iint \left[ \dot{n}_{A}(z) \Delta \mu_{A} - \dot{n}_{B}(z) \Delta \mu_{B} \right] dydz \qquad (2.13)$$
  
where  $\Delta \mu_{A} = \mu_{A} - \mu_{AE}$  and  $\Delta \mu_{B} = \mu_{B} - \mu_{BE}$ . The actual limits of

integration in the y direction are arbitray because the integrand is a function of z only. Integration of Eq. 2.13 over an

$$-T\dot{S}_{p} = \int \left[ \Delta \mu_{A} \dot{n}_{A}(z) \delta y - \Delta \mu_{B} \dot{n}_{B}(z) \delta y \right] dz \qquad (2.14)$$

The total mass transfer is equal to the integration of the mass flux over the interfacial area

$$\dot{N}_{A} = \int \dot{n}_{A}(z) \, dy \, dz \tag{2.15}$$

Since the mass flux is independent of y, taking the derivative of Eq. 2.15 gives

$$\frac{dN_A}{dz} = n(z)\delta y \qquad (2.16)$$

Substitution of Eq. 2.16 into Eq. 2.14 yields

$$-T\dot{S}_{p} = \int \Delta \mu_{A} d\dot{N}_{A} - \int \Delta \mu_{B} d\dot{N}_{B}$$
(2.17)

Assuming constant molal overflow (12) the mass flow rate of component A must be related to the mass flow rate of component B

$$\dot{dN}_{A} = \dot{dN}_{B}$$
(2.18)

Equation 2.17 can now be simplified to

$$-T\dot{S}_{p} = \int \left[ \Delta \mu_{A} - \Delta \mu_{B} \right] d\dot{N}_{A}$$
(2.19)

The differences in chemical potential, at constant pressure and temperature may be expressed as (15)

$$\Delta \mu_{A} = RT \ell n \frac{y_{A}}{y_{AE}}$$
(2.20)

$$\Delta \mu_{\rm B} = RT \, \ell n \frac{y_{\rm B}}{y_{\rm BE}} \tag{2.21}$$

Equation 2.19 can now be rearranged to yield

$$\dot{s}_{p} = R \int \ell n \left[ \frac{y_{E}(1-y_{A})}{y_{A}(1-y_{AE})} \right] \dot{dN}_{A}$$
 (2.22)

where the identities  $y_A + y_B = 1$  and  $x_A + x_B = 1$  have been used to simpligy the result.

A mass balance on component A of the bulk vapor flow gives (12)

$$d\dot{N}_{A} = \overline{V}dy_{A}$$
(2.23)

where  $\overline{V}$  is the bulk vapor molar flow rate and dy<sub>A</sub> is the change of component A of the bulk vapor. Substitution of Eq. 2.23 into Eq. 2.22 produces the needed equation for total entropy production due to mass transfer in a binary system

$$S_{p} = \overline{VR} \int_{y_{A,in}}^{y_{A,out}} ln \left[ \frac{y_{AE}(1-y_{A})}{y_{A}(1-y_{AE})} \right] dy_{A}$$
 (2.24)

The parameters controlling the rate of entropy production in the tower are now obvious; the vapor flow rate  $\overline{V}$  (a function of the reflux ratio), the inlet and outlet mole (or mass) fractions, and the relationship between  $y_A$  and  $y_{AE}$  (a function of the reflux ratio and the relative volatility).

Two important points need to be mentioned. First, as the mole fraction,  $y_A$ , approaches the equilibrium mole fraction,  $y_{AE}$ , the integrand approaches zero. Thus the point of minimum entropy production coincides with that of minimum reflux. Second,  $y_{AE} > y_A$  guarantees that the argument of the logarithm cannot be less than unity, which means that  $\dot{S}_p > 0$ .

## 2.3 Application to Simple Tower Design

# 2.3.1 System Description

Consider a simple distillation system (Figure 2.2) designed to process 700 lbm/hr (318 kgmol/hr) of feed (16). The unit is to operate continuously for 8500 hrs/yr at a total pressure of one atmosphere. The feed contains 45 mol % benzene and 15% toluene. The feed is saturated at its boiling temperature of 201°F(94°C). The objective of this separation process is to divide the feed into two product streams; an overhead product consisting of 92% benzene and a bottoms containing 95% toluene. Table 2.1 lists additional information about this system. The distillation tower is a continuous contactor having a packing material cost of \$38/ft<sup>3</sup>. The purchase costs for tower shell, condenser, and reboiler were obtained from manufacturer's data based on weight for the shell and area for the heat exchangers. The sum of piping, insulation, and instrumentation etc. are taken to be 60% of the cost for the installed equipment. The steam supplied to the reboiler is saturated at 292°F and is priced at  $$0.75/10^3$  lbm, and the cooling water is priced at \$0.045/10<sup>3</sup> gal.

# 2.3.2 Available-Energy Analysis

Using standard techniques (17,18) an available-energy analysis was performed on the system operating at a reflux ratio of 1.2, and shows the overall Second-Law efficiency to be 12.9% (19). The relevant equations for this analysis are given in Table 2.2. The reboiler has a Second-Law efficiency equal to



Figure 2.2. Schematic diagram of the binary distillation system. The available energy flows and consumptions are given in  $10^6$  Btu/hr.

#### TABLE 2.1

#### SYSTEM DESIGN INFORMATION

2.5 Relative volatility,  $\alpha$ Molal heat capacity of 40.0 Btu/lbmol<sup>o</sup>F the liquid mixture, C Molal heat of vaporization of mixture, h 13700 Btu/lbmol Heat transfer coefficient of 80 Btu/hr  $ft^{2}$  °F the reboiler, hr Heat transfer coefficient of 100 Btu/hr ft<sup>2</sup> °F the condenser, h Initial AT of condenser cooling 50 <sup>o</sup>F 90 <sup>o</sup>F water Inlet cooling water temperature Inlet state of steam saturated vapor at 60 psia Heat of condensation of steam 915.5 Btu/lbm Boiling temperature of feedstock 201 °F 92% benzene Overhead product purity 95% toluene Bottoms product purity Feed composition 45% benzene 700 lbmol/hr Feed flow rate

#### TABLE 2.2

# AVAILABLE-ENERGY BALANCE EQUATIONS

$$\begin{split} \hat{\Delta A}_{st} &= \hat{Q}_{rb1r} \left[ 1 - \frac{T_0 s_{fg}}{h_{fg}} \right] \\ \hat{A}_{D,rb1r} &= T_0 \dot{s}_{p,rb1r} = \frac{T_0 \dot{Q}_{rb1r} \left[ T_{st} - T_{pr} \right]}{T_{st} T_{pr}} \\ \hat{\Delta A}_1 &= \Delta \dot{A}_{st} - \dot{A}_{D,rb1r} \\ \hat{A}_{D,cond} &= T_0 \dot{s}_{p,cond} = \dot{m}_{cw} c_{cw} T_0 \left[ \ell n \frac{T_3}{T_0} - \frac{T_3 - T_0}{T_{cond}} \right] \\ \hat{A}_3 &= \dot{m}_{cw} c_{cw} T_0 \left[ \frac{T_{out}}{T_{in}} - 1 - \ell n \frac{T_{out}}{T_{in}} \right] \\ \hat{A}_2 &= -\dot{A}_3 + \dot{A}_{D,cond} \\ \hat{A}_{D,co1} &= T_0 S_{p,cond} = \overline{V} R T_0 \int_{y_{A,in}}^{y_{A,out}} \ell n \left[ \frac{y_{AE}(1-y_A)}{y_A(1-y_{AE})} \right] dy_A \\ \dot{A}_{f \rightarrow p} &= \Delta \dot{A}_1 + \Delta \dot{A}_2 - \dot{A}_{D,co1} \end{split}$$
$\Delta\dot{A}_{1}/\Delta\dot{A}_{st}$  or 74.2%. The tower efficiency, defined as  $\Delta\dot{A}_{f \rightarrow p}/(\Delta\dot{A}_{1}+\Delta\dot{A}_{2})$ is 55.7%. Note that it is of little use to evaluate a condenser efficiency without consideration of the system as a whole inasmuch as the role of the condenser is to rid the system of low-temperature heat (entropy). The tower available-energy destruction was computed using Eq. 2.24. It is interesting to note that the value for  $\Delta\dot{A}_{feed \rightarrow product}$  computed above compares closely to the calculated value for the isothermal minimum work of separation, 0.36(10<sup>6</sup>) Btu/hr, (12). The small difference in these two results arises from assumptions made in evaluating the consumption of available energy in the tower.

## 2.3.3 Thermoeconomic Governing Equations

The objective of design optimization is the selection and/or specification of system hardware which minimizes the total expenditure for capital, fuel, and other costs (20,21). The use of an explicit Second Law design strategy enables a large complex system to be split into much less complex parts. Each subsystem can then be optimized individually. The primary advantage of such an approach is the additional insight gained by dealing with much simpler systems.

The basis of any thermoeconomic analysis is the application of a money balance to the system or subsystem of interest

$$\$_{\text{product}} = \Sigma \$_{\text{fuel}} + \Sigma \$_{\text{capital, etc.}}$$
 (2.25)

The cost of the product of an energy conversion system must equal the sum of fuel expenses and capital (and labor ....)

charges. It is often convenient to express the product cost in terms of the average unit cost of product,  $\lambda_p$ , and the total amount of product,  $P_p$ , or  $\$_{product} = \lambda_p P_p$ . Similarly the fuel costs may be expressed as  $\$_{fuel} = \lambda_f P_f$ . Equation 2.25 may now be written as

$$\lambda_{p} = \frac{\sum_{p}^{\lambda} f^{p} f}{P_{p}} + \frac{\sum_{capital}^{s} f^{capital}}{P_{p}}$$
(2.26)

The first term in this equation reflects fuel costs and, alternatively could be expressed in terms of the system inefficiencies and the system utility costs. The second term is indicative of the capital investment. However, the system inefficiencies and the capital investment are functions of the design variables. Thus minimization of the unit cost of product involves a function that is dependent on only the utility or fuel costs and the design variables.

The strategy to be employed in this chapter requires the application of a money balance to each system component. That is, each system component is viewed as an energy converter which processes fuel from one form to another and sends its product along to the next system component for further processing. Then, beginning with a "working design" each system component is optimized for minimum unit product cost. These suboptimizations are done successively for each component in an iterative fashion until the design converges. This procedure requires the use of available energy as the measure of thermodynamic value for fuel inputs and product outputs (20). In the system of interest the reboiler transfers some of the available energy in steam to the bottoms stream. The column uses the increase in available energy of the bottoms to transform feed into products. The condenser processes the reflux for subsequent re-use in the column. In the boiler and column available energy is supplied in one form and converted into a product. However, the condenser exists for the sole purpose of decreasing the available energy of the reflux. Or in other terms, the condenser serves to eliminate entropy from the system.

This however complicates the optimization procedure somewhat. The problem can be alleviated by using an entropy penalty function,  $\dot{P}_s$ , which serves to properly apportion the total condenser costs to the reboiler and column. The entropy penalty function, which has been called "negentropy" (22,23), can also be viewed as the commodity or product which the condenser sells to the tower and reboiler. The entropy penalty function leaving the condenser is given by (19,23,24)

 $\dot{P}_{s,cond} = \dot{Q}_{cond} - T_0 \dot{S}_{p,cond} - \dot{A}_{net exit,cond}$  (2.27) The entropy penalty function attributable to the reboiler is given by (19)

$$\dot{P}_{s,reboiler} = \frac{T_0}{T_1} \dot{Q}_{rblr}$$
(2.28)

and the entropy penalty function attributable to the column is found by difference

$$P_{s,col} = P_{s,cond} - P_{s,rblr}$$
(2.29)

Thus by requiring the reboiler and column to purchase  $P_{s, rblr}$ ,  $P_{s, col}$  from the condenser, the condenser costs are properly included in the optimization procedure. However, the money balances will need to include the money flows associated with the entropy penalty function transactions.

Essentially the column is viewed as a system through which the circulating process stream is converted to product streams. The circulating process stream passes through the reboiler and condenser extracting and depositing available energy. From this perspective it is only reasonable to price the process stream at a constant cost  $\lambda$ , which is analogous to the extraction method (25). This constant price  $\lambda$ , obtained from the reboiler money balance, is used to cost the inefficiencies in both the tower and the condenser.

A money balance on the reboiler yields

$$\lambda \Delta A_{1} = \lambda_{st} \Delta A_{st} + Z_{rb1r} + \lambda_{s} P_{s,rb1r}$$
(2.30)

where  $\lambda$  represents the cost of the circulating process stream,  $\lambda_{st}$  is the unit cost of steam,  $\dot{Z}_{rblr}$  is the capital cost of the reboiler, and  $\lambda_s$  is the unit cost of the entropy penalty function. Similarly a money balance on the condenser gives

$$\lambda_{s} \dot{P}_{s,cond} = \lambda \Delta \dot{A}_{2} + \lambda_{cw} \dot{m}_{cw} + \dot{Z}_{cond}$$
 (2.31)

However, with the aid of an available energy balance (see Table 2.2) Eq. 2.31 can be rearranged to yield

$$\lambda_{s}\dot{P}_{s,cond} = \lambda T_{0}\dot{S}_{p,cond} + \lambda \dot{A}_{cond,exit}$$

$$+ \lambda_{cw}\dot{m}_{cw} + \dot{Z}_{cond}$$
(2.32)

where  $\lambda$  represents the cost of the circulating process stream flowing between the column and condenser and  $T_0 \dot{s}_{p,cond}$  is the available energy destruction in the condenser.

Equations 2.31 and 2.32 can be solved for  $\lambda$  and  $\lambda_{s}$ 

$$\lambda = \frac{\lambda_{st} \Delta \dot{A}_{st} + \dot{z}_{rblr} + (\lambda_{cm} \dot{m}_{cw} + \dot{z}_{cond}) \frac{P_{s,rblr}}{\dot{P}_{s,cond}}}{\Delta \dot{A}_{1} - \left[T_{0} \dot{S}_{p,cond} + \dot{A}_{cond,exit}\right] \frac{\dot{P}_{s,rblr}}{\dot{P}_{s,cond}}$$
(2.33)

and

$$\lambda_{s} = \frac{\lambda_{cw} \hat{m}_{cw} + Z_{cond} + \lambda T_{0} S_{p,cond} + \lambda \dot{A}_{cond,exit}}{\dot{P}_{s,cond}}$$
(2.34)

A money balance on the tower yields

$$\lambda_{\rm p} = \frac{\lambda (\dot{\Delta A_1} + \dot{\Delta A_2}) + \lambda_{\rm s} \dot{P}_{\rm s, col} + \dot{Z}_{\rm col}}{\dot{\Delta A}_{\rm f \rightarrow p}}$$
(2.35)

Equations 2.33-2.35 are the basic thermoeconomic governing equations for the Second Law based optimization.

## 2.3.4 Optimization Procedure

Given a set of design variables (a working design), capital cost equations as functions of the design variables (19), the unit costs of utilities, and Eqs. 2.33-2.35 the Second-Law based optimization may be performed.

The first step in this procedure is to perform an analysis of a working design of the system in order to obtain values for the unit cost of the process stream,  $\lambda$ , and the entropy cost penalty function,  $\lambda_{s}$ . In turn unit cost are used to optimize the column.

The first subsystem to be optimized is the column. Given a set of specified product purities and column pressure the reflux ratio remains as the only column variable, that is,  $\lambda_p$  is a function of reflux ratio. Using values for  $\lambda$  and  $\lambda_s$  obtained from the analysis of the working design,  $\lambda_p$  is computed from Eq. 2.35 for several values of reflux ratio (Table 2.3). The optimal reflux ratio is obtained via a search of these values.

The next component to be optimized is the reboiler. The reboiler area is fixed once the values for steam temperature,  $T_{st}$ , and process stream temperature,  $T_1$ , are fixed (assuming a constant heat transfer conductance). The process stream temperature is fixed by the column pressure and the product purities.

Thus only  $T_{st}$  remains as a variable. The unit cost of the process stream,  $\lambda$ , is then optimized via Eq. 2.33 with respect to the steam temperature (Table 2.3).

The last component to be optimized is the condenser. The condenser area is fixed once the process stream temperature,  $T_2$ , and the exit cooling water temperature,  $T_3$ , are fixed. However, the process stream temperature is fixed by the column pressure and the product purities. Thus the condenser is optimized by minimizing the unit cost of the entropy penalty function  $\lambda_s$ , with respect to  $T_3$ .

The result of these procedures is a new set of design variables as well as a new set of unit product costs,  $\lambda_p$ ,  $\lambda$ , and  $\lambda_s$ . The above procedure is then repeated until the design variables and unit

costs converge. It is the author's experience that for simple systems convergence is usually attained in one or two iterations. The computer software needed to perform these tasks is included in Appendix B.

## 2.4 Results and Conclusions

The principle results of applying this Second Law based design methodology to the previously described separation system are contained in Table 2.3. In addition, the results of applying a traditional method - that of a direct search through the design space - are also presented in Table 2.3. As can be seen, both methods yield an optimum reflux ratio equal to 1.20. More detailed results are given in Reference 19.

The results presented in Table 2.3 show that as the capital investment in the tower  $(Z_{tower})$  increases at higher tower heights, the available energy destruction decreases. Thus the optimal design reflects the classical trade-off between capital investment and fuel cost. It is important to note that heat exchanger design plays a major role in separation systems (26). At the optimum reflux ratio, the reboiler and condenser represent 21% and 12% of the total capital investment. Similarly at the optimum design the fuel costs, steam and cooling water, represent 64% and 8% of total system costs.

The fundamental advantage of the Second Law methodology is the fact that the optimization of a complex separation system is greatly simplified by breaking up the system into its individual components and individually suboptimizing each one in order to achieve a global optimum.

Reflux Ratio	Column Height (Diameter) (ft)	Column Available Energy Consumption (105 Btu/hr	Column Cost (10 <sup>3</sup> \$/yr)	Reboiler Cost (10 <sup>3</sup> \$/yr)	Condenser Cost (10 <sup>3</sup> \$/yr)	Steam Cost (10 <sup>3</sup> \$/yr)	Cooling Water Cost (10 <sup>3</sup> \$/yr)	Second-Law Based Unit Product Cost (\$/106 Btu)	Unit Product Cost Obtained from a Direct Search Method (\$/10 <sup>6</sup> Btu)
1.14	37(7.43)	2.54	23.7	5.93	3.51	66.5	8.66	37.64	37.71
1.16	32 (7.47)	2.59	21.4	5.97	3.53	67.1	8.74	37.13	37.19
1.18	30(7.50)	2.64	20.2	6.00	3.55	67.7	8.82	37.00	37.03
1.20	28.5(7.54)	2.70	19.4	6.03	3.56	68.3	8.90	37.00	37.00
1.25	25.7(7.63)	2.84	18.2	6.11	3.61	69.8	9.11	37.28	37.22
1.30	23.9(7.72)	2.98	17.4	6.19	3.66	71.4	9.31	37.63	37.61
1.40	21.4(7.89)	3.26	16.5	6.35	3.75	74.5	9.71	38.85	38.60
1.60	18.7(8.23)	3.82	15.8	6.66	3.93	80.6	10.52	41.43	40.94
1.80	17.2(8.55)	4.38	15.6	6.92	4.11	86.7	11.33	44.19	43.43
2.00	16.1(8.86)	4.95	15.5	7.18	4.30	92.9	12.14	47.03	46.0

TABLE 2.3 RESULTS OF SECOND LAW OPTIMIZATION

The number of variables in this simple system is not large enough to preclude traditional methods. The three optimizing variables are the steam condensing temperature, the reflux ratio, and the cooling water exit temperature. The product purities were assumed fixed by market demands and the column pressure was fixed at one atmosphere. In the separation of multicomponent mixtures (more than two components) there are multiple distillation columns and many different configurations are possible. Because of the complexity of multicomponent separation systems traditional optimization techniques are very tedious and therefore heuristic methods (sometimes involving many rules-of-thumb) are employed to choose the best configuration. The application of the Second Law design methodology promises to reduce the number of variables involved as well as to provide the designer with greater insight because one is working with each system component on an individual basis.

## 2.5 Closure

This work has provided a framework for further application of Second Law based design methodology to complex separation systems. It has done so by providing a relationship that gives the available energy destruction in a binary separation tower as a function of the process variables. The Second Law methodology has been described and applied to a simple binary separation system. The method yields results identical to those obtained from a traditional direct search method, and accurately indicates the respective trade-offs between fuel costs and capital investment.

# 3. COGENERATION AND THE LAGRANGE METHOD OF SYSTEM OPTIMIZATION

## 3.1 Cogeneration

In years past, when fuel costs were low and represented only a small fraction of the total system cost, the design and purchasing practice was almost entirely regulated by trying to minimize capital investment. In today's economy, the philosophy of minimizing total cost must include fuel and maintenance as they represent a significant portion of total cost. This philosophy places a much higher value on efficiency and equipment reliability and accepts the additional capital investment required provided that there is economic justification based on future payback. The net result is an increase in the performance of systems, leading to improved energy productivity (product output per unit of energy input) and greater conservation of resources.

In order to increase energy productivity the concept of energy cascading is receiving greater acceptance. Energy cascading refers to the matching of the quality (temperature) of an energy source (the available energy) to the requirements of the task. This concept is realized by combined cycles and cogeneration systems.

Cogeneration has been utilized by industry for many years but recent trends in purchased fuel and power costs have significantly influenced the economics of cogeneration to a more favorable position. This method of producing low temperature heat has an advantage over the more conventional system of burning fuel for low temperature applications in

that a cogeneration system has a lower available energy destruction than the conventional system. In other words, cogeneration systems can provide low temperature heat at higher Second Law efficiencies than the alternative of producing low temperature steam from a low pressure boiler or furnace. (27-30)

Figure 3.1 represents an industrial-sized Rankine cycle cogeneration system where steam bled off the turbine at intermediate and lower pressures provides the required energy for the low temperature heating. The turbine is particularly useful because it can supply heat at a range of temperatures by selecting the stage from which the steam is bled. The outlet pressure and temperature from a cogeneration system's boiler are generally much higher than dictated by the low temperature heating requirement so that the available energy losses due to heat transfer in the alternative low pressure boiler are reduced by passing the high temperature steam through a turbine to obtain shaft work.

Cogeneration systems produce two vastly different products. The thermal energy produced is generally in the form of low pressure steam or hot water. The shaftwork produced is generally used directly in some process or used to produce electricity. There is some question as to the proper characterization of these products so to provide a consistent basis for comparison. From Figure 3.1 we can see that the energy and available energy produced in the form



Figure 3.1. Available Energy and (Energy) Analysis for an Industrial Rankine Cycle Cogeneration System

of shaftwork are equal at ten units, but the thermal product, steam, contains seventy-five units of energy and only twenty units of available energy. To characterize these product streams by their energy content does not take into account the usefulness of each product.

From a fuel conservation standpoint, cogeneration systems are extremely effective thermal systems and their potential economic advantages keep them as an ever growing part of the world's energy usage. Traditionally, many cogeneration systems have been designed where either the electricity or thermal energy is treated as the principle product and the other is treated as a by-product which must be used on site or wasted. When the electricity is considered the principal product the cogeneration system can be designed to track the electric demand. This presents problems in the utilization of the thermal product. Fluctuations in the system's electrical output will cause fluctuations in the thermal output and unless the electrical and thermal demands are well matched, the system will waste some of the thermal energy.

Continuous operation of the cogeneration system is particularly applicable when the thermal energy is considered the principal product. The relatively invariant thermal demands of some industries lend themselves to a system which will track the thermal demand. Historically low electric/ thermal ratios have been used so that the plant could use all the electricity produced and would purchase the balance of its electrical needs from the utility.

In 1978 Congress passed the Public Utility Regulatory Policies Act (PURPA). This act requires utilities to purchase all excess electricity produced by cogenerators at <u>the full</u> <u>cost avoided by the utility</u> while providing back up or standby power at the same retail rates charged to non-cogenerating customers having similar load profiles. This recent development (pending litigation) provides additional incentives for cogeneration by allowing more flexibility in the design of the cogeneration system. With the assurance of grid interconnection and backup power, tracking thermal loads no longer has the restriction of low electric/thermal ratios. Systems may now be designed without the concern that any electricity produced in excess of its own needs will be wasted. This has enhanced the prospect for cogeneration by improving the

economics for both large and small scale systems.

Power systems such as liquid and gas-fired Diesel, Otto and Brayton cycles can now be more frequently used for cogeneration. These systems generally have high electric/ thermal ratios and are advantageous for small scale cogeneration applications because they can accommodate large fluctuations in output (even frequent shut downs). PURPA has thus created an entirely new market for cogeneration in the small business and residential sectors. Cogenerators can choose to increase production or even to come online only when electricity is most expensive. The cost of electricity produced by utilities varies both seasonally and hourly. If cogenerators can coordinate their thermal load with peak electric prices, the electricity that they produce becomes much more valuable.

Rankine cycle cogeneration systems are generally applicable to situations where a constant demand for low temperature heat is present. The integration of steam turbines into industrial energy systems is not a new concept. It is a practice which has been used by many industries as an economical method of supplying shaft power, electricity, and process heat as well as making use of waste heat rejected by many processes. Industries for which Rankine cycle cogeneration systems are particularly well suited include the chemical, petroleum, refining, paper and pulp, metals and mining, and food industries.

District heating is another use for Rankine cycle cogeneration systems. When power stations are located near business or population centers, it may be economical to

supply them with low temperature thermal energy. The thermal energy is generally transported in the form of steam in the United States and in the form of hot water in Europe. Pipelines connect the power station and consumers where the circulated steam or hot water is used for space heating and for the production of domestic hot water.

The United States was the pioneer in the practical application of district heating and about forty such units are currently in operation. Denmark and Sweden are using this concept extensively with Denmark producing thirty-five percent of all its heat requirements in this manner.

Cogeneration systems represent investments with an economic life ranging from thirty to forty years. The economics of cogeneration are highly dependent on the local relative prices of fuel and electricity. Existing systems have demonstrated that for many current economic situations, cogeneration systems can yield a profitable return on investment now, and as fuel and purchased electricity prices rise, profits will increase. The net effect of cogenerating is a conservation in capital and fuel as well as a reduction in air and thermal pollution.

## 3.2 Optimization Procedure Using Lagrange's Method

Thermal systems can be completely described using balance equations for mass, energy, and entropy in conjunction with thermophysical property relations and/or equations of state, equipment performance characteristics, thermokinetic or rate equations, and boundary/initial conditions. With the

thermal system adequately described, it can be optimized using Lagrange's Method of Undertermined Multipliers. Although such a description is not explicit in Second Law terms, the method will yield the same optimal design and with the appropriate transformations, will yield any desired Second Law quantity.

The variables which are used to describe the system usually are not all independent since there exist equations of constraint. It may be possible to substitute the constraint equations into the objective function, leaving only independent variables to be optimized. Unfortunately, it is not always mathematically possible or desirable to eliminate all the dependent variables from the objective function. One alternative is the use of Lagrange's Method of Undetermined Multipliers (See Appendix C).

El-Sayed and Tribus discuss and application of Lagrange's Method to the design of a simple gas turbine system (31). The method requires the objective function to be expressed in terms of the dependent (or state) variables,  $x_i$ , and independent (or decision) variables,  $y_k$ .

$$\phi_{0} = \phi_{0} (\{x_{i}\}, \{y_{k}\})$$
(3.1)

The equations of constraint are divided into two groups. One set of constraints, referred to as <u>substitution constraints</u>, are used to eliminate selective dependent variables from the objective frunction,  $\phi_0$ , and from the set of Lagrange

constraints,  $\phi_j$ . The other set of constraints, <u>called</u> <u>Lagrange constraints</u>, are used directly in the optimization scheme, each having an associated Lagrange multiplier,  $\lambda_j$ . These constraints are defined by equations of the form

$$\phi_{i} = \phi_{i} - x_{i} \tag{3.2}$$

where  $\phi_j$  is the equation of constraint to be used in Lagrange's Method (a Lagrange constraint). The constraint must be equal to zero at the optimum,  $\phi_j$  is the defining equation that describes the relation between the associated state variable,  $\{x_j\}$ , and the other state variables,  $\{x_{i\neq j}\}$ , and decision variables  $\{y_k\}$ , and where  $x_i$  is a state variable typically associated with an available energy flow.

With these definitions, the Lagrange constraints are then expressed as functions of the state and decision variables

$$\phi_{j} = \phi_{j}(\{x_{i}\}, \{y_{k}\}) \qquad j = 1,n$$
 (3.3)

Using this approach, the problem is formulated

Extremize 
$$\phi_0 = \phi_0 (\{x_i\}, \{y_k\})$$
 (3.4)

Constrained by  $\phi_{j} = \phi_{j} (\{x_{i}\}, \{y_{k}\}) \quad j = 1, n$  (3.5)

With the selection of the objective function and Lagrange constraints, the Lagrangian, L, is defined by

$$L = \phi_{0} + \sum_{j} \lambda_{j} \phi_{j}$$
(3.6)

In accordance with the Method of Lagrange, to guarantee that L is independent of the set of state variables,  $\{x_i\}$ (i.e. L is unconstrained or in other words, that the optimum of L is equal to the constrained optimum of  $\phi_0$ ), we must have

$$\frac{\partial L}{\partial x_i} = 0 \quad i = 1, n \tag{3.7}$$

or

$$\frac{\partial \phi_{0}}{\partial x_{i}} + \sum_{j=1}^{n} \lambda_{j} \frac{\partial \phi_{j}}{\partial x_{i}} = 0 \quad i = 1, n \quad (3.8)$$

This yields a set of n equations which are linear in the unknown Lagrangian multipliers,  $\{\lambda_j\}$ . Equations 3.8 may be put in matrix form and rearranged to yield

$$\left\{\frac{\partial \phi_{j}}{\partial x_{i}}\right\} \quad \left\{\lambda_{i}\right\} = -\left\{\frac{\partial \phi_{o}}{\partial x_{i}}\right\} \quad (3.9)$$

or

$$\{\lambda_{i}\} = - \left\{\frac{\partial \phi_{0}}{\partial x_{i}}\right\} \quad \left\{\frac{\partial \phi_{j}}{\partial x_{i}}\right\}^{-1}$$
(3.10)

The Lagrangian multipliers may be interpreted as prices which reveal the economic value associated with a differential change in the corresponding state variables, and are referred to as shadow prices (31).

When the objective function and Lagrange constraints are well behaved analytic functions, the optimum design is defined by

$$\left\{\frac{\partial \mathbf{L}}{\partial \mathbf{y}_{k}}\right\} = \left\{0\right\}$$
(3.11)

or rewriting Eq. 3.11

$$\left\{ \frac{\partial \phi_{0}}{\partial y_{k}} \right\} + \left\{ \lambda_{i} \right\} \left\{ \frac{\partial \phi_{i}}{\partial y_{k}} \right\} = \left\{ 0 \right\}$$
 (3.12)

The optimum design is therefore located by solving the resulting simultaneous equations to obtain each optimum decision variable,  $y_k$ .

When optimizing real world problems it is often convenient to define a marginal price,  $\theta_k$ , associated with each decision variable,  $y_k$ . The set of marginal prices are defined

$$\theta_{k} = \frac{\partial L}{\partial y_{k}}$$
(3.13)

$$= \frac{\partial \phi_{0}}{\partial y_{k}} + \sum_{i=1}^{n} \lambda_{i} \left( \frac{\partial \phi_{i}}{\partial y_{k}} \right)$$
(3.13a)

k = 1, m

$$\left\{\theta_{k}\right\} = \left\{\frac{\partial L}{\partial y_{k}}\right\} = \left\{\frac{\partial \Phi_{o}}{\partial y_{k}}\right\} + \left\{\lambda_{i}\right\} \left\{\frac{\partial \Phi_{i}}{\partial x_{i}}\right\}$$
(3.14)

The physical interpretation of these marginal prices is that they are prices associated with a differential change in the corresponding decision variables,  $\{y_k\}$ , and may be used to indicate the potential benefit of changing a decision variable.

Matrix Eq. 3.10 represents n linear equations in the unknown Lagrangian multipliers and Eq. 3.14 represents m simultaneous equations with the decision variables as unknowns. Note that each shadow or marginal price may be expressed as the ratio of two determinants (See Appendix D), each containing the derivatives of the objective function and the Lagrange constraint equations. These determinants, called Jacobians, can be written as

$$J\{A_{j}\} = J\left\{\frac{\phi_{1}, \phi_{2}, \dots, \phi_{j-1}, \phi_{0}, \phi_{j+1}, \dots, \phi_{n}}{x_{1}, x_{2}, \dots, x_{j-1}, x_{j}, x_{j+1}, \dots, x_{n}}\right\}$$
(3.15)

$$J\{B\} = J \left\{\frac{\phi_1, \phi_2, \dots, \phi_n}{x_1, x_2, \dots, x_n}\right\}$$
(3.16)

$$J\{C_{k}\} = J\left\{\frac{\phi_{1}, \phi_{2}, \dots, \phi_{n}, \phi_{0}}{x_{1}, x_{2}, \dots, x_{n}, y_{k}}\right\}$$
(3.17)

Now, each shadow and marginal price may be expressed as

$$\lambda_{j} = -J\{A_{j}\}/J\{B\}$$
 (3.18)

$$\lambda_{j} = -J \left\{ \frac{\phi_{1}, \phi_{2}, \dots, \phi_{j-1}, \phi_{0}, \phi_{j+1}, \dots, \phi_{n}}{\phi_{1}, \phi_{2}, \dots, \phi_{j-1}, \phi_{j}, \phi_{j+1}, \dots, \phi_{n}} \right\}$$
(3.19)

$$= - \left(\frac{\partial \phi_{0}}{\partial \phi_{i}}\right) \qquad (3.19a)$$

and

 $\theta_{k} = J\{C_{k}\}/J\{B\}$  (3.20)

or

$$\theta_{k} = J \left\{ \frac{\phi_{1}, \phi_{2}, \dots, \phi_{n}, \phi_{0}}{\phi_{1}, \phi_{2}, \dots, \phi_{n}, y_{k}} \right\}$$
(3.21)

$$= \left(\frac{\partial \phi_{0}}{\partial y_{k}}\right) \qquad (3.21a)$$

For many practical applications of this method, the n+k equations corresponding to Eqs. 3.10 and 3.14 are highly non-linear and quite unwieldy to solve. Consequently, a numerical solution may be necessary. One such procedure is to obtain numerical values for the shadow prices,  $\{\lambda_i\}_{\ell}$ , from Eq. 3.10 for a particular set of design variables,  $\{\lambda_k\}_{\ell}$ . These shadow prices are then introduced to Eq. 3.14 and the marginal prices,  $\{\theta_k\}_{\ell}$ , evaluated. The marginal prices represent the derivatives of the objective function,  $\phi_0$ , at that particular design point,  $\ell$ . It is then possible to use the marginal prices to point in the direction toward the optimum design. The new set of design variables,  $\{y_k\}_{\ell+1}$  is determined using



Figure 3.2 Graphical Interpretation of a Negative Marginal Price



Figure 3.3 Graphical Interpretation of a Positive Marginal Price

$$y_{k,\ell+1} = y_{k,\ell+\Delta yk}$$
(3.22)

or

$$y_{k,\ell+1} = y_{k,\ell-\Delta yk}$$
(3.23)

where  $\Delta y_k$  is some predetermined interation increment.

When the marginal price,  $\theta_{k,l}$ , is negative the derivative of the objective function is negative. If we wish to minimize the objective function, this indicates that the decision variable needs to be increased in order to approach the optimum, and Eq. 3.22 should then be used. Similarly, if the marginal price,  $\theta_{k,l}$ , is positive, the decision variable needs to be decreased in order to approach the optimum, so that Eq. 3.23 should then be used.

In many cased it is informative to have Second Law based prices associated with a change in thermodynamic value streams corresponding to  $\theta_k$  or  $\lambda_i$ . These Second Law based prices may be obtained by using the chain rule

$$\lambda_{s} = \lambda_{i} \left( \frac{\partial \mathbf{x}_{i}}{\partial A} \right) = \lambda_{i} \left( \frac{\partial A}{\partial \mathbf{x}_{i}} \right)$$
(3.24)

$$\theta_{s} = \theta_{k} \quad \left(\frac{\partial y_{k}}{\partial A}\right) = \theta_{k} \left(\frac{1}{\partial A}\right) \quad (3.25)$$

where  $\lambda_s$  and  $\theta_s$  are prices associated with changes in an available energy stream, A (which has  $y_k$  and  $x_i$  as variables),

through changes in  $y_k$  and  $x_i$ . A non-dimensional marginal price,  $e_k$ , is often desired. This is accomplished using Eq. 3.26.

$$\Theta_{k} = \Theta_{k} \left( y_{k} / \phi_{0} \right)$$
(3.26)

#### 3.3 Closure

This chapter has reviewed the principles of cogeneration which appears to be a most promising and growing energy conservation measure. Cogeneration will become particularly attractive if pending litagation and legislation does not alter the fundamental thrust of the 1978 Public Utility Regulatory Policies Act (PURPA), which requires electric utilities to purchase all excess electricity <u>at the</u> full avoided cost to the utility.

In addition, this chapter reviews the fundamental equations for application of Lagrange's Method to the optimal design of thermal systems. Essentially the Lagrange Method is a rational technique which allows the engineer to study the effect of changes in design variables on the overall system design.

#### 4. OPTIMIZATION OF A RANKINE CYCLE COGENERATION SYSTEM

4.1. Introduction

There is a great thermodynamic advantage to employing a cogeneration system. However a system's real potential must be proven in the marketplace. In order to demonstrate the economic value of a cogeneration system one must compare the cost of its products to that of products produced by a different means.

The alternative to a cogeneration system is usually taken as a low pressure boiler or furnace which supplies the necessary thermal energy and purchasing the electricity from a utility. Comparing the economics of this type of system to the optimally designed cogeneration system will indicate the potential benefit of cogeneration.

In order to locate the optimal design for a cogeneration system, the requirements of the system must be known. Most industrial plants have the option of purchasing electricity from a utulity or producing some or all of its electrical needs, also, PURPA makes it possible for cogenerators to sell electricity to the utility.

This provides a great deal of flexibility in the amount of electricity that can be produced. The heat required for process is usually inflexible. Generally, the processes which use the thermal energy have rigid requirements on the amount of energy necessary and the temperature at which it must be delivered.

The optimization must focus on how much shaft work (or electricity) the cogeneration system should produce, given a specific product heat requirement, for present and future market conditions. The optimization must simultaneously locate the optimal capital investments, performance specifications, and operating characteristics for the system.

Lagrange's Method of Undetermined Multipliers is particularly well suited for many engineering applications and may be applied to cogeneration systems. Specifically, this method will be applied to a Rankine cycle cogeneration system in a fashion similar to that of Tribus and El-Sayed's work on gas turbine design (31).

The working fluid for the Rankine cycle is steam, the properties of which are usually available in tabular or graphical form. This suggests that a completely analytical solution is not desirable and that a numerical technique should be employed.

The cogeneration system consists of four major components, boiler, turbine/generator, condenser and boiler feed pump.

The system produces two products, electricity and base load hot water. The hot water produced is the exiting cooling water from the condenser/heat exchanger. This means that the steam must condense at a relatively high temperature and pressure since it is the condensing steam which supplies the required available energy to the hot water.



Figure 4.1. Rankine Cycle Cogeneration System

The hot water is supplied to process at a high temperature, TB, and is returned at a lower temperature, TC. The supply and return temperatures are specified by the process and are therefore treated in the optimization as constants.

The approach selected to optimize the system is that of suboptimizing the system at various fixed electrical outputs. This will yield an optimal design for each specified electrical output. These suboptimizations will not be functions of the price of electricity and will depend only on the relative cost of fuel and equipment, and the cost of capital. Once the value of

electricity is known, the overall optimum design can be selected from these suboptimizations.

The problem must be set up such that the objective function and the Lagrange constraint equations are functions of the state and decision variables.

$$\phi_{0} = \phi_{0} [\{x_{i}\}, \{y_{k}\}]$$
(4.1)

$$\phi_{j} = \phi_{j} [\{x_{j}\}, \{y_{k}\}]$$
(4.2)

A major deviation from the procedure followed by Tribus and El-Sayed (31) is in the selection of the Lagrange constraint equations and state variables. The added complexity of having steam as the working fluid (compared to an ideal gas in the gas turbine problem) makes it impractical to select state variables that correspond to available energy flows. Because this requirement could not be rigidly adhered to, it was relaxed entirely. This gives the designer the opportunity to use any variable as a state variable. This allows considerably more freedom in the selection of state and decision variables which in turn simplifies the objective function, Lagrange constraint equations, and subsequent derivatives.

#### 4.2. Objective Function

The optimization of the cogeneration system at constant work output is a problem which has fixed products as a requirement. This allows the objective of the optimization to be stated

Minimize the total cost of owning and operating the system (at fixed products).

The objective function is then expressed in terms of the system's costs (fuel, equipment, and capital) by using an amortized capital investment, Z, for each component and the total fuel cost, CFUEL, written on a per operating hour basis. The objective function may be written as

#### 4.3. Cost Estimation

The capital costing equations used in the cogeneration problem have been designed to yield approximate capital and maintenance expenditures and to reflect the consequence of changing the system's variables on these costs. The form of these equations express equipment costs in terms of steam and performance variables. In all cases a capital recovery factor, CRF, is used to account for the cost of capital, i, and estimated useful life, n, which puts costs on a per year basis.

CRF (i,n) = 
$$\frac{i(1+i)^n}{(1+i)^n - 1}$$
 (4.4)

For an interest rate of fifteen percent, a useful life of forty years, and an operating time of eight thousand hours per year, the capital recovery factor on a per operating hour basis is

$$CRF(15,40) = \frac{0.15 (1.15)^{40}}{(1.15)^{40} - 1} * \frac{1}{8000} = 1.875 \times 10^{-5}$$
(4.5)

The approach taken in the development of these costing equations was to single out the most important parameters which influence cost, and use them to yield a base cost, designating them with a prime (i.e. Z'). This base cost is then adjusted by multiplication factors so as to incorporate the influence of other factors. The form of these equations has been suggested in the literature and by experienced engineers, then curve fit to available data (31-38). However, extreme care must be exercised when applying any of these equations in the field.

## 4.3.1. Boiler Costing Equation

The boiler investment was found to be primarily a function of the steam mass flow rate (STM), outlet pressure (P1) and the boiler pressure drop (AR) and First Law boiler efficiency (AN). The mass flow rate and outlet pressure are used to give the base cost. This cost plots linearly on log-log paper and may be expressed using the relation

$$\log_{10} ZB' = (A+B*P1) + C * \log_{10} STM$$
 (4.6)

where

A = 1.3043876  $B = 6.128129 \times 10^{-4}$  C = 0.7718955  $[STM] = [1b_m/hr]$  [P] = [psia] [Z'] = [\$]

Solving for the base cost

ZB' = Cll [exp (Bll\*Pl)][exp (Bl2\* aLog STM)] (4.7) where

 $C_{11} = \exp (A + (a \log 10)) = 20.1552224$   $B_{11} = B^*(a \log 10) = 1.4110546 \times 10^{-3}$  $B_{12} = C = 0.7718795$ 

The boiler oulet pressure determines the intercept of the line and since the slope is constant, it effectively choose the appropriate line. The mass flow rate then determines the point along the line which yields the base cost. This base cost incorporates the cost associated with tube diameter and thickness, and the use of alloys as required for the specified mass flow rate and pressure.

The effects of First Law boiler efficiency, pressure drop, and outlet steam temperature on the estimated cost are incorporated through the use of multiplication factors. The boiler shell side pressure drop factor, FAR, is designed to show the influence of tubing size (length, arrangement, etc.) on the boiler. As with all other multiplication functions, FAR is designed so that it can be easily adjusted to fit current data. This can be done by changing the constants in these factors, in this case the reference pressure loss coefficient, ARS, and the shape constant, B15

FAR = 1.0 + [(1.0-ARS)/(1-AR)]\*\*B15 (4.8)
Figure 4.3 shows the value of the multiplication factor, FAR,
as a function of pressure loss coefficient, AR, for values of



Figure 4.2. Base Boiler Cost Versus Steam Mass Flow Rate the reference pressure loss coefficient, ARS = 0.92 and shape constant B15 = 8.0.

A similar expression is used to describe the effect of First Law efficiency on boiler cost. This multiplication factor, FAN, is expressed as

$$FAN = 1.0 + [(1.0-ANS)/(1.0-AN)]**B14$$
 (4.9)

For a reference efficiency, ANS, of 0.90 and a shape constant of 7.0, the function, FAN appears as in Figure 4.4. This



Figure 4.3. Boiler Pressure Drop Factor Versus Boiler Pressure Drop Coefficient



Figure 4.4. Boiler Efficiency Factor Versus Boiler Efficiency

function increases gradually until state-of-the-art efficiencies are reached where the additional capital investment required to improve efficiency increases dramatically.

The boiler outlet temperature was not found to be a measure of boiler cost until metallurgical limits were reached. As this temperature approaches  $1050^{\circ}$ F, boiler maintenance costs begin to increase drastically due to accelerated creep rates (39). The boiler temperature factor, FAT, is designed to reflect this quickly escalating cost.

$$FAT = 1.0 + C12 * exp [(T1-T1S)/B13]$$
 (4.10)

This multiplication factor appears in Figure 4.5 at a reference temperature, T1S, of  $1100^{\circ}$ F and for shape constants C12 = 5, and B13 = 18.75.



Figure 4.5. Boiler Temperature Factor Versus Temperature

## 4.3.2. Turbine-Generator Costing Equations

Turbine-generator costs were found to be mainly a function of the turbine's shaft work output (WA), turbine inlet and outlet steam conditions, generator efficiency, and turbine isentropic efficiency (BN). The generator efficiency is considered a fixed parameter not to be optimized, thus it does not appear explicitly in the developed costing equation. The base cost is determined from the expression

$$ZB' = C21 * exp \{B21 * ln [FB1 * (F2T+F2P)]\}$$
(4.12)

$$FB1 = B22 * BN * STM$$
 (4.13)

$$F2T = CPS (T1R-T2R-T2R*ln (T1R/T2R))$$
 (4.14)

$$F2P = R*T2R*ln (P_1/P_2)$$
 (4.15)

$$B22 = 3.929119 \times 10^{-4}$$

$$C21 = 5.240378 \times 10^{3}$$

$$TIR = T1(^{\circ}F) + 460 = (^{\circ}R)$$

$$T2R = T2(^{\circ}F) + 460 = (^{\circ}R)$$

$$CPS = 0.55 (Btu/lb_m^{\circ}F)$$

$$R = 0.1102 (Btu/lb_m^{\circ}F)$$

B21 = 0.569323

where

This base turbine cost reflects the nearly logarithmically linear relationship between turbine shaft work and cost yet it also accounts for variations of turbine cost as a function of inlet and outlet steam conditions. In addition to this base cost, the influence of turbine isentropic efficiency and inlet steam temperature is assessed through multiplication factors FBN and FBT, respectively. The gas turbine isentropic efficiency function, FBN, is given by

$$FNB = [(1.0-BNS)/(1.0-BN)]**B24$$
(4.16)

where

$$BNS = 0.95$$

B24 = 3.0

This function is plotted in Figure 4.6 and is designed to account for increasing turbine costs associated with increasing isentropic efficiency. Note the gradual increase in the function over the feasible range followed by a sharp increase as state-ofthe-art efficiencies are approached and surpassed.

The effect of temperature on the creep rate of the turbine blades is sharply exponential beginning at 1050°F. This sharply increases maintenance costs as temperatures approach this mark. These costs are reflected in the temperature multiplication factor, FBT, shown in Figure 4.7. This function is designed to have very little effect until temperatures are reached at which creep becomes a problem.

$$FBT = 1.0 + C22 \exp[(T1-T1S)/B23]$$
(4.17)

where


Figure 4.6. Turbine Isentropic Efficiency Factor Versus Turbine Isentropic Efficiency





T1S =  $1100^{\circ}$ F C22 = 5.0 B23 = 18.75

## 4.3.3. Condenser Costing Equations

The parameter which the condenser's base cost is most influenced by is the heat transfer area, CA. The base cost is divided into two distinct segments. For heat transfer areas between one hundred and three thousand square feet, condenser cost per unit area is closely logarithmically linear when plotted versus heat transfer area. The base cost in this range can be expressed as

ZC' = CA\*C31\*exp(B31\*ALog CA) (4.18)  
for 100 
$$\leq$$
 CA  $\leq$  300 ft<sup>2</sup>

where

C31 = 426.2632633B31 = -0.4556513

For areas greater than three thousand square feet, condenser base cost is proportional to heat transfer area

$$ZC' = CA + C36$$
 (4.19)  
for CA > 3000 ft<sup>2</sup>

where

$$C36 = 1.11$$
  
[CA] = [ft<sup>2</sup>]

Adjustments to this base cost were made for shell and tube side pressure losses and for condenser operating pressure. The multiplication factors for pressure drop are taken from Tribus and El-Sayed (31). The steam side (shell side) pressure drop factor, FCR, is given by

$$FCR = P3 * ((1/CR)-1)/C35 **B32$$
 (4.20)

and is illustrated in Figure 4.8.

The water side (tube side) pressure drop factor, FCPW, is also plotted in Figure 4.8 and is given by



Figure 4.8. Shell and Tube Side Pressure Loss Factors Versus Pressure Loss

where

```
C35 = 14.7
B32 = -0.38
B33 = -0.11
```

The condenser operating pressure effect on cost is estimated by using a second order polynomial curve fit. This factor, FCP, is shown in Figure 4.9 and is given by

$$FCP = C32 + C33 * P2 + C34 * (P2**2)$$
 (4.22)

where

C32 = 0.930  $C33 = 2.6380952 \times 10^{-4}$   $C34 = 1.352381 \times 10^{-6}$ [P] = [psia]

The condenser costing equation also contains the function FCB (see Figure 4.10). This function is designed as an inequality constraint, effectively establishing the minimum temperature difference allowed in the condenser (in this case it was set at  $5^{\circ}$ F). The slope of this function is steep near the five degree mark but is zero elsewhere. The optimization scheme uses the evaluation of derivatives as the basis for iteration. This function does not significantly effect the cost estimate or optimization scheme for large temperature differences because its value is one and derivative zero. On the other hand, when the minimum temperature difference approaches  $5^{\circ}$ F the optimization technique will not allow the iteration to proceed because of the

(4.21)



Figure 4.9. Condenser Pressure Factor Versus Condenser Pressure



Figure 4.10. Condenser Temperature Factor Versus Minimum Temperature Difference

large value of the derivative. This function may be expressed as

$$FCB = \exp(B34/(T2-TB-5))$$
(4.23)

where

B34 = 0.10

### 4.3.4. Pump Costing Equations

Included in pump costs is the expense associated with the starter and electric motor. These costs are found mainly to be influenced by work input to the pump (WP) and by the pump efficiency (DN). The costing trend associated with input is in the form of a logarithmically linear function. This base cost, illustrated in Figure 4.11, is given by

$$ZD' = C41 \exp(B41*a\log[B42*STM*V34*(P4-P3)/DN])$$
(4.24)

where

C41 = 1969.2325B41 = 0.4838546 B42 = 7.2709088x10<sup>-5</sup> V34 = 0.018

The effect of efficiency on cost can be incorporated in the costing equation through the use of the factor FDN (Figure 4.12) which is given as

$$FDN = 1 + ((1 - DNS) / (1 - DN)) **B43$$
 (4.25)

where

DNS = 0.80B43 = 3.00



Figure 4.11. Pump Base Cost Versus Pump Work



Figure 4.12. Pump Isentropic Efficiency Factor Versus Pump Isentropic Efficiency

BOILER	ZA ZA		ZA(STM, P1, T1, AN, AR) X11 * FAP * FAM * FAT * FAN * FAR
where	X11 FAP FAM FAT FAN FAR		CRF * Cll exp(Bl1 * Pl) exp(Bl2 * alog STM) 1.0 + Cl2 * exp[(T1-T1S)/Bl3] 1.0 + [(1.0-ANS)/(1.0-AN)]**Bl4 1.0 + [(1.0-ARS)/(1.0-AR)]**Bl5
TURBINE & GENERATOR	ZB ZB		ZB(STM, P1, P2, T1, T2, BN) X21 * FBW * FBT * FBN
where	TIR T2R X21 FB1 F2T F2P FBW FBT FBN		T1 + 460 T2 + 460 CRF * C21 B22 * BN * STM CPS * (T1R-T2R-T2R*alog(T1R/T2R)) R * T2R * alog (P1/P2) exp{B21 * alog [FB1 * (F2T+F2P)]} 1.0 + (C22 * exp [(T1-T1S)/B23]) 1.0 + [(1.0-BNS)/(1.0-BN)]**B24
CONDENSER	ZC ZC		ZC(CA, P3, P2, PB, PC, T2, TB) X31 * FCA1 * FCR * FCPW * FCP * FCB
for	100	4	$CA \leq 3000 \text{ ft}^2$
	ZC	=	X31 * FCA2 * FCR * FCPW * FCP * FCB
for	CA	>	3000
where	X31 FCA1 FCA2 FCR FCPW FCP FCB		CRF CA * C31 * exp(B31 * alog CA) CA * C36 [P3 * ((1/CR)-1.0)/C35]**B32 [(PC-PB)/C35]**B33 C32 + C33 * P2 + C34 * (P2**2) exp(B34/(T2-TB-5))
PUMP	ZD ZD	=	ZD(STM, P4, P3, DN) X41 * FD1 * FDN
where	X41 Y2 FD1 FDN		CRF * C41 B42 * STM * V34 * (P4-P3)/DN exp[B41 * alog Y2] 1.0 + [(1.0-DNS)/(1.0-DN)]**B43
FUEL	CFUEI	.=	CF * HF

Table 4.1. Amortized Costing Equations for the Cogeneration System

## 4.3.5. Fixed Charges

The costing equations previously discussed determine the cost associated with each component of the system. The total system cost is composed of the sum of the component consts (ZTOT) plus any other charges attributable to the system. These other charges, called fixed charges, include such costs as the piping between components, foundation charges, building charges, operating personnel charges, etc. Fixed charges are estimated at 1.5 times the sum of the component costs. These costs are considered constant for a specified heat and work output requirement. Because the Lagrange optimization scheme is at fixed product, these costs need not be incorporated into this part of the optimization. However, these charges must be considered in order to select the optimum work/heat ratio from the set of suboptimizations (each at constant product).

### 4.4. Optimization Procedure

The equations of constraint link the cost estimate through the system's thermodynamic performance to fuel costs. The thermodynamic analysis must interrelate the variables used to describe the system's performance to those used in the cost estimate. In this problem, costing equations are used which are almost entirely in terms of steam and performance variables. Thus the thermodynamic analysis need only be in terms of these variables.

In order to determine the constraints, it is necessary to examine the thermodynamics of the cycle. The state points

of the steam cycle are given in Figure 4.13 in temperatureentropy coordinates. Sixteen equations of constraint have been developed from a thermodynamic analysis of the cycle, and are given in Table 4.2.

Some constraints, such as  $\phi_2$ , use stream variables to describe the thermodynamic state of the working fluid. Numerical values for steam properties are generated using a computer subroutine called STEAM (40). Thus not all constraint equations are in analytical form.

The selection of fixed parameters and decision variables are found in Table 4.3.

The problem has now been reduced to five independent variables. The form of the constraints have been arranged



Figure 4.13. Steam Cycle for the Cogeneration System in T-S Coordinates

State Variable x <sub>i</sub> =		THERMODYNAMIC CONSTRAINTS Defining Relation <sup>\$\delta\$</sup>						
н2	=	f(P2,X2)	1					
т2	=	f(P2, two phase)	2					
P3	=	P2 * CR	3					
HЗ	=	f(P3, SAT.L)	4					
P4	=	P1/AR	5					
H4	<del></del>	H3 + CF1 * V34 * (P4-P3)/DN	6					
STM	=	HWM * CPW * (TB-TC)/{CN*(H2-H3)}	7					
WP	-	STM * (H4-H3)	8					
Hl	=	(WA+WP)/STM + H2	9					
<b>T</b> 1	=	f(H1, P1)	10					
H2S	-	f(P1,P2,T1)	11					
BN	=	(WA+WP)/(STM * (H1-H2S))	12					
HF	=	STM * (H1-H4)/AN	13					
Т3	=	f(P3, SAT. L)	14					
TM	=	{(T3-TC) - (T2-TB)}/alog{(T3-TC)/(T2-TB)}	15					
CA	=	HWM * CPW * (TB-TC)/(TM*U)	16					

Table 4.2. Equations of Constraint for the Cogeneration System

Lagrange Constraints

 $\phi_{i} = \phi'_{i} - x_{i}$  i = 1,16

# Table 4.3. Fixed Parameters and Decision Variables for the Cogeneration System

## ${y_f}$ FIXED PARAMETERS

TB	Condenser hot water outlet temperature
TC	Condenser hot water inlet temperature
PB	Condenser hot water outlet pressure
PC	Condenser hot water inlet pressure
HWM	Required hot water mass flow rate
WA	Net turbine shaft work output
CR	Condenser shell-side pressure loss coefficient
X2	Turbine exit quality
U	Condenser overall heat transfer coefficient
CPW	Specific heat of water at constant pressure
CN	Condenser First Law efficiency
$\{y_k\}$	DECISION VARIABLES
AN	Boiler efficiency
AR	Boiler pressure drop coefficient
P1	Turbine inlet pressure
P2	Condenser inlet pressure
DN	Pump isentropic efficiency

such that each state variable can be solved for explicitly and the order selected such that the resulting matrix is diagonalized. The next step is to obtain equations for the solution of the shadow and marginal prices. This requires the evaluation of various derivatives of the constraint equation matrix. However, because not all the constraints are in algebraic form (those constraints that are functions of steam table properties), numerical derivatives must be evaluated. One other note, there are two condenser costing equations. This means that two separate derivatives must be taken and the derivative corresponding to whichever costing equation is valid for that value of condenser area, is the one which should be used.

The shadow prices are determined using Eq. 3.10. Simply stated, the j-th shadow price,  $\lambda_j$ , is determined by taking the derivative of the Lagrangian (Eq. 3.6) with respect to the j-th state variable  $x_j$ . Setting this equal to zero yields

$$\frac{\partial \mathbf{L}}{\partial \mathbf{x}_{i}} = \frac{\partial}{\partial \mathbf{x}_{i}} \left[ \phi_{0} + \sum_{i} \lambda_{i} (\phi_{i}' - \mathbf{x}_{i}) \right] = 0.$$
(4.26)

This can be rearranged to yield

$$\frac{\partial}{\partial \mathbf{x}_{j}} \left[ \phi_{0} + \sum_{i \neq j} \lambda_{i} (\phi_{i} - \mathbf{x}_{i}) \right] = - \frac{\partial}{\partial \mathbf{x}_{j}} \left[ \lambda_{j} (\phi_{j} - \mathbf{x}_{j}) \right]$$
(4.27)

Because  $\phi_j$  is not a function of  $\mathbf{x}_j$  the right hand side reduces to

$$-\frac{\partial}{\partial x_{j}} [\lambda_{j}(\phi_{j} - x_{j})] = \lambda_{j}$$
(4.28)

Furthermore, the left hand side can be simplified by noting that the  $\frac{\partial x_i}{\partial x_j}$  terms are equal to zero. Thus with these modifications the shadow price  $\lambda_i$  can be written as

$$\lambda_{j} = \frac{\partial}{\partial \mathbf{x}_{j}} \begin{bmatrix} \phi_{o} + \sum_{i \neq j} \lambda_{j} \phi_{j}^{'} \end{bmatrix}$$
(4.29)

which corresponds to the equation represented as one row of Eq. 3.10. For example, application of Eq. 4.26 to solve for the third Lagrange multiplier, SP(3) (Shadow Price 3), yields

$$SP(3) = \frac{\partial}{\partial P3} \phi_0 + \sum_{i=1}^{2} SP(i)\phi'_i + \sum_{i=4}^{16} SP(i)\phi'_i$$
(4.30)

Inspection of the costing constraints indicates that CFUEL, ZA, and AB are independent of P3 and therefore those derivatives are zero. A similar inspection of the Lagrange constraints shows only  $\phi'_4$ ,  $\phi'_6$ , and  $\phi'_{14}$  to have dependence on P3. Equation 4.30 can now be simplified to

$$SP(3) = \frac{\partial}{\partial P3} [ZC + ZD + SP(4) \phi'_{4} + SP(6)\phi'_{6} + SP(14)\phi'_{14}]$$
(4.31)

The first term involves the condenser costing equations. This means derivatives must be taken using the corresponding costing equation which is applicable for that particular value of condenser area. The two condenser costing equations differ only by the factors FCA1 and FCA2, thus derivatives of the other multiplication factors will be identical. Both condenser costing equations depend on P3 in the same manner through the factor FCR.

$$\frac{\partial}{\partial P3} [FCR] = \frac{\partial}{\partial P3} \left[ \left( \frac{P3\left(\frac{1}{CR} - 1\right)}{C35} \right)^{B32} \right] = \frac{FCR * B32}{P3}$$
(4.32)

After some algebraic manipulation (see Appendix E) the two derivatives become

$$\frac{\partial}{\partial P_3} \left[ ZC(100 \le CA \le 3000) \right] = ZC \quad \frac{(100 \le CA \le 3000) *B32}{P_3}$$
(4.33)

$$\frac{\partial}{\partial P3} \left[ ZC(CA > 3000) \right] = \frac{ZC(CA > 3000) *B32}{P3}$$
(4.34)

In this case the two expressions are algebraically identical except for the costing equation which was used to evaluate the condenser cost, therefore, only one equation will be necessary so long as the correct value of CA is used. In the general case, separate equations must be determined and the correct one selected. The next term of Equation 4.31 involves the pump cost estimate.

$$\frac{\partial}{\partial P_3}$$
 [ZD] = x<sub>11</sub>\*FDN \*  $\frac{\partial}{\partial P_3}$  [FD1] (4.35)

but

$$\frac{\partial}{\partial P3} [FD1] = - \frac{FD1*B41}{(P4-P3)}$$
(4.36)

so

$$\frac{\partial}{\partial P3} \left[ ZD \right] = - \frac{ZD * B41}{(P4 - P3)}$$
(4.37)

The term involving  $SP(6)*\phi_6'$  is straightforward, with the Lagrange multiplier SP(6) treated as a constant, yielding

$$\frac{\partial}{\partial P3} \left[ SP(6) * \phi_{6}^{\prime} \right] = SP(6) * \frac{\partial}{\partial P3} \left[ \phi_{6}^{\prime} \right]$$
$$= - \frac{SP(6) * DF1 * V34}{DN}$$
(4.38)

The other two terms to be evaluated contain constraints which use the computer subroutine STEAM for solution. This means numerical derivatives must be taken using the increment, DP3. These two terms may then be evaluated as

$$\frac{\partial}{\partial P_3} [SP(4) * \phi_4] = SP(4) * \frac{H_3(P_3 + DP_3, SAT.L) - H_3(P_3, SAT.L)}{DP_3}$$
  
= SP(4) \* DER3 (4.39)

$$\frac{\partial}{\partial P3}$$
 [SP(14)\* $\phi_{14}$ ] = SP(14) \*  $\frac{T3(P3+DP3, SAT.L) - T3(P3, SAT.L)}{DP3}$ 

$$=$$
 SP(14) \* DER4 (4.40)

where DER3 and DER4 are dummy variables used to store the value of the numerical derivative.

One expression can be used for the third shadow price.

+ SP(14)\*DER4

$$SP(3) = \frac{ZC*B32}{P3} - \frac{ZD*B41}{(P4-P3)} + SP(4)*DER3 - \frac{SP(16)*CF1*V34}{DN}$$
(4.41)

This equation appears with the other shadow price equations in Table 4.5. In a similar fashion, all sixteen shadow prices are evaluated (see Appendix E for details). It is easiest to keep track of the necessary derivatives using a matrix as in Table 4.4. Because the constraints are diagonalized the shadow price matrix is an upper diagonal matrix. (In a similar fashion the marginal price matrix will also be an upper diagonal.) The solution for the shadow prices is listed in Table 4.5.

Marginal prices are evaluated using Eq. 3.11 and 3.12. Again it is easiest to keep track of these derivatives by using a matrix such as in Table 4.6.

# Table 4.4. Shadow Price Matrix for the Cogeneration System

Solution Vector	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
¢0		×	×		×		×			×		×	×	1		×
SP(16) (\$16-CA)															×	×
SP(15)(\$15-TM)		×												x	x	
$SP(14)(\phi_{14}^{-T3})$														×		
SP(13)(\$13-HF)						x	x		×				x			
SP(12) (\$12-BN)							X	×	×		×	×				
SP(11) ( + H2S)										×	×					
SP(10)(\$10-T1)		1							×	×						
SP(9)(¢ <sub>9</sub> -H1)	×						X	×	×							
SP(8)(0,-WP)				×		×	X	×								
SP(7)(\$7-STM)	x			×			x						1		-	
SP(6)(46-H4)			×	×	×	x										
SP(5)(\$5-P4)					×											
SP(4)(44-H3)			x	×												
SP(3)(\$3-P3)			×													
SP(2)(\$2-T2)		×									1					
SP(1)(¢1-H2)	x															
	e 3HZ	<u>ar2</u>	e BP3	e H3	9 <u>P4</u>	9H4	e	e	e BHI	e JTI	a BH2S	e 9BN	a HF	e eTG	e WLE	9CA

X indicates that a derivative must be taken. O or blank indicates no entry or a zero value.

## Cogeneration System SP(16) = (ZC/CA)\*(B31+1)for $100 \leq CA \leq 3000 \text{ ft}^2$ SP(16) = (ZC/CA) $CA > 3000 \text{ ft}^2$ for SP(15) = -SP(16)\*CA/TM $SP(14) = SP(15)*{(alog DUM1)-1+1/DUM1}/{alog(DUM1)}*2$ SP(13) = CFSP(12) = X21\*FBT\*FBW\*[FBN\*B21/BN+(FBN-1)\*B24/(1-BN)]SP(11) = SP(12)\*BN/(H1-H2S)\*\* SP(10) = SP(11)\*DER1+X11\*FAP\*FAN\*FAR \*FAM\*(FAT-1)/B13+X21\*FBN \*FBW\*[(FBT-1)/B23+FBT\*B21 \*CPS\*(1-T2R/T1R)/(F2T+F2P)] \*\*SP(9) = SP(10)\*DER2-SP(12)\*BN/(H1-H2S)+SP(13)\*STM/AN SP(8) = [SP(9)+SP(12)/(H1-H2S)]/STMSP(7) = [SP(8)\*WP-SP(9)\*(WP+WA)/STM-SP(12)\*BN+SP(13)\*HF+ZA\*B12+ZB\*B21+ZD\*B41]/STM SP(6) = SP(8)\*STM-SP(13)\*STM/AN SP(5) = SP(6)\*CF1\*V34/DN+ZD\*B41/(P4-P3) SP(4) = SP(6)+SP(7)\*STM/(H2-H3)-SP(8)\*STM \*\*SP(3) = SP(4)\*DER3-SP(6)\*CF1\*V34/DN+SP(14) \*DER4+ZC\*B32/P3-ZD\*B41/(P4-P3) SP(2) = SP(15)\*[-alog(DUM1)+DUM1-1]/[alog(DUM1)]\*\*2+ZB\*B21\*[-CPS\*alog(T1R/T2R)+R\*alog(P1/P2)] /(F2T+F2P)-ZC\*B34/(T2-TB-5)\*\*2 SP(1) = -SP(7)\*STM/(H2-H3)+SP(9)

Shadow Price Equations for the

\*DUM1 = (T3-TC)/(T2-TB)

Table 4.5.

DER = numerical derivative number \_\_\_\_.

Marginal Price	(T) W4	PM(2)	(E) M4	(4) Md	PM(5)
ф <sub>о</sub>	×	×	×	×	×
SP(16) 016					
SP(15) 015					
$SP(14)\phi_{14}$					F.
SP(13) 013	×	-			
SP(12) ¢ 12			-		
SP(11) 011			x	×	
SP(10) 010			×		
SP(9) 09					
SP(8) 08					
SP(7) \$					
SP(6) \$		×			
SP(5) \$			x		x
$SP(4)\phi_4$					
SP(3) ¢3				X	
SP(2) 02				Х	
SP(1) •				×	
	e	e	9 171	<del>3</del> 172	9 AR

Table 4.6. Marginal Price Matrix for the Cogeneration System

X indicates that a derivative must be taken. O or blank indicates no entry or a zero value. For example,  $\phi_{13}$  and  $\phi_0$  are the only functions which depend on the decision variable AN. The associated marginal price, PM(1), is

$$PM(1) = \frac{\partial}{\partial AN} \left[ SP(13) * \phi_{13} + \phi_0 \right]$$
(4.42)

$$PM(1) = SP(13) \frac{\partial}{\partial AN} [\phi'_{13}] + \frac{\partial}{\partial AN} [ZA]$$
(4.43)

$$PM(1) = -SP(13) * HF/AN + X11 * FAP * FAM *$$

FAT \* FAR \* (FAN-1) \* 
$$B41/(1-AN)$$
 (4.44)

The marginal price equations can all be easily solved because of the diagonalization. The marginal price equations are listed in Table 4.7. For a detailed derivation see Appendix E.

The solution procedure requires the designer to select a feasible set of decision variables  $\{y_k\}$  for the first iteration. Once this initial set of five decision variables has been chosen, the entire design (for that iteration) is fixed and the set of state variables  $\{x_i\}$ , and cost estimates are determined. With values assigned to all the state and decision variables, the set of shadow prices,  $\{SP(i)\}$ , are evaluated, then in turn, the set of marginal prices,  $\{PM(i)\}$ , are determined. These marginal prices are then used to

	Table 4.7.		Marginal Pric Cogeneration	for the		
PM(1	) =	-SP(13)*	HF/AN+X11*FAP	*FAM*FAT*FAR*	(FAN-1)*B14/(1-AN)	
PM(2	) =	-SP(6)*() *B43/(1-)	H4-H3)/DN+X41; DN]	*FD1*[-FDN*B4	1/DN+(FDN-1)	
*PM(3	) =	SP(5)/AR R*T2R/[P	+SP(10)*DER5+5 1*(F2T+F2P1]	5P(11)*DER6+2	A*B11+ZB*B21*	
**PM(4 for	) =	DUM2+DUM 100 ≤ CA	3*FCA1 ≤ 3000 ft <sup>2</sup>			
**PM(4 for	) =	DUM2+DUM CA > 300	3*FCA2 0 ft2			
PM(5	) =	-SP(5)*P (FAR-1)*1	1/AR**2+X11*FA B15/(1-AR)	AP*FAM*FAT*FA	N*	

\*DER\_ = numerical derivative number \_\_\_.
\*\*DUM2 = SP(1)\*DER7+SP(2)\*DER8+SP(3)\*CR+SP(11)\*DER9
 -ZB\*B21\*R\*T2R/(P2(F2T+F2P))

DUM3 = X31\*FCP\*FCR\*FCPW\*FCB\*(C33+2\*C34\*P2)

direct the iteration as described by Eq. 3.22 and 3.23. The computer program used to optimize the system is given in Appendix F and results and recommendations presented in the next chapter.

#### 5. RESULTS OF COGENERATION OPTIMIZATION

## 5.1 Computer Program Operation and Application

A computer program (Appendix F) was developed to optimize the cogeneration system discussed in Chapter 4. The program is arranged such that the main program is little more than an executive routine that calls seven subroutines which perform the mathematical computations.

The first subroutine, called VALUE, initializes the constants, fixed parameters, and the set of decision variables. The constants and some fixed parameters are assigned values directly by the program while the value of other fixed parameters (HWM, TC, TB, WA) must be input by the user. This subroutine also accepts the initial values for the decision variables.

Subroutine CONSTR evaluates the thermodynamic constraints (found in Table 4.2) solving for the sixteen state variables which correspond to that set of decision variables. Once all the variables have been assigned values, subroutine COST estimates the associated capital costs, and subroutines SHADOW and MARGIN evaluate the shadow and marginal prices for that design.

Subroutine NEWVAL uses these marginal prices to generate a new set of decision variables (according to Eq. 3.22 and Eq. 3.23). This subroutine operates in one of two modes. When a particular set of decision variables is far from the optimal set, there will be a large difference in the total

operating cost between two successive iterations. This difference can be used as a measure of the distance from the optimum. When the difference is large, the entire set of decision variables is changed based on the input set of marginal prices. When the difference is smaller than some present value, only one decision variable is changed and a new set of state variables, shadow prices, and marginal prices are evaluated. Using this new set of marginal prices, another decision variable is changed and a new set of marginal prices computed. This is automatically repeated until all the decision variables have been changed. Each time a complete set of new decision variables is generated, the program displays the parameters necessary to evaluate the system design. The user must then respond whether or not he wishes to iterate again. When the design is adequate, the program stores the optimal system parameters in a file. An example of the program output is shown in Appendix F.

This program can be used to generate a variety of data. It is possible to parametrically vary any or all of the fixed decision variables. The parameters which were varied are CF, W/Q and TB (see Table 5.1). The stratagem was to monitor the change in the optimal design by changing fuel cost and work output for several hot water requirements. In this manner, given the economic conditions and hot water requirements, the optimal amount of shaft work can be selected from these suboptimizations.

Stu
ßtı

1.00

## Table 5.1. Parametrically Varied Fixed Variables for the Cogeneration System

## 5.2 Results of Suboptimizations

Appendix G contains the important optimal system parameters for each of the suboptimizations. Inspection of this data shows some interesting trends in the optimal system design. It is important to note that all trends are highly dependent on the costing equations.

The trends in stream and performance variables associated with increasing fuel costs are that of increasing the system's performance. As the cost of fuel rises the boiler efficiency, pump isentropic efficiency, and turbine isentropic efficiency all increase. The condenser's thermodynamic performance increases because the steam's condensing temperature (or pressure as can be seen in Figure 5.3) decreases, approaching the required hot water temperature. This general increase in performance allows the steam mass flow rate, boiler pressure and pump work all to decrease. As an example of this increase in the system's performance, Figure 5.1 and Figure 5.2 clearly show the increase in boiler efficiency and pump isentropic efficiency associated with the increasing fuel costs for different values of the work/heat ratio.

This increase in system performance is not free. The incremental economic benefit of decreased fuel consumption is balanced by the incremental increase in the required capital investment. This is apparent from Table G.2 (Appendix G), where the required capital investment for









each component (and hence the system) consistently increases as fuel costs rise.

The one decision variable which remains relatively unaffected by the cost of fuel is the boiler pressure drop coefficient, AR. This decision variable seems to decrease slightly or remain stable as fuel costs rise. This seems to indicate that the effect of the boiler pressure drop, AR, is dominated by the benefit which can be gained by altering other system parameters.

The magnitude of the change in some system parameters associated with increasing fuel costs is small. From a practical standpoint, these changes in the optimal parameters may even be of little engineering significance. For example, when the required hot water temperature, TB, equals 250°F and the work/heat ratio is 0.175, the pump efficiency, DN, goes from 0.665 to 0.670 as fuel costs go from two to four dollars per million Btu, however, over the same range, the condensing temperature, T2, changes from 262.2°F to 260.5°F which may be significant in the design of the condenser.

More significant trends occur as the work/heat ratio increases. Varying this parameter is extremely important in order to locate the optimal work output given a specific heat requirement and fuel cost. Trends in the system parameters and costs associated with changing work/heat ratio are plotted in Figures 5.1 and 5.7.

The effect of the work/heat ratio, W/Q, on the optimal boiler efficiency, BN, is that of decreasing BN as W/Q increases. This is an interesting trend because its justification may not be immediately apparent. For low work/heat ratios the condenser (and hence its products) play a dominating role in the design of the system. The condenser has a specific energy requirement which the boiler must supply. The energy supplied to the stream (hence the First Law or boiler efficiency) is very closely tied to the condenser. The shaft work produced by the turbine is dependent not only on the amount of energy supplied by the boiler but also on the temperature and pressure at which it is supplied. In other words, the shaft work is dependent on the available energy input to the turbine. Thus for larger shaft work outputs, one needs to increase boiler pressure and to a lesser extent temperature, that is an increase in the boiler Second Law efficiency. However, the boiler efficiency is predominantly a function of temperature (assuming that the superheated steam behaves ideally). Therefore, for larger values of the work/heat ratio, the turbine dominates and requires a large available energy input from the boiler. This may be accomplished by an increase in the boiler exit pressure and temperature which is not fully reflected in boiler efficiency. On the other hand, when the condenser dominates it requires a larger heat input to the working fluid and thus a maximum boiler efficiency regardless of the boiler outlet pressure.

Figure 5.2 shows the isentropic pump efficiency plotted versus the work/heat ratio. There is an upward trend for pump efficiency as the work/heat ratio rises. This is because the increased pressure demanded by the turbine requires additional pump work. The pump's increased importance in the system therefore calls for improved performance (efficiency). This same trend is shown in Figure 5.2 for several different fuel costs and for two different required hot water temperatures.

Two ways of increasing the amount of shaft work produced (at fixed Q) are (1) to decrease the turbine outlet pressure, P2, and/or (2) to increase the turbine inlet pressure, Pl. These two effects are clearly demonstarted in Figures 5.3 and 5.4. Figure 5.3 shows how the optimum turbine outlet pressure decreases as the amount of work produced increases. These curves drop steeply until pressures are reached which correspond to condensing temperatures near the 255°F mark (TB+5°F). The condenser cost factor, FCB, prevents the temperature from going below this mark. The optimal values for the turbine inlet and outlet pressures are determined with the optimization balancing the incremental pump, boiler, and turbine costs resulting from the increasing of Pl against the incremental condenser and turbine cost associated with lowering P2.

The boiler pressure drop coefficient increases as the work/heat ratio increases. This is clearly demonstrated in Figure 5.5. As the shaft-work becomes more important in



Figure 5.3 Optimum Condenser Inlet Pressure Versus Work/Heat Ratio



Figure 5.4 Optimum Turbine Inlet Pressure Versus Work/Heat Ratio

the system, improved system design tends in the direction of decreasing the pump work by lessening the pressure drop in the boiler.

The system's Second Law efficiency rises as the work/ heat ratio increases (as shown in Figure 5.6). This is partially due to improved performance of the turbine, pump, and condenser and the higher temperature steam from the boiler. This considerably decreases the available energy destruction due to heat transfer in the boiler. Thus, the turbine can take advantage of this for the production of shaft-work.

Altering TB (holding TC and HWM constant) changes the amount of heat which must be supplied to the hot water, Q. When comparing the thermodynamic stream and performance variables for various TB, it is then important that a comparison be made for the same value of the work/heat ratio. It must be kept in mind that the scale of the systems being compared is different.

Increasing the required hot water temperature, TB, implies the turbine outlet pressure (temperature) must also increase. This means that for the same work/heat ratio, the turbine inlet pressure must also be higher as is clearly demonstrated by Figure 5.4. Other trends associated with increasing TB include the decreasing of the maximum temperature difference in the condenser, an increase in pump efficiency (Figure 5.2), and an increase in the system's Second Law efficiency.



Figure 5.5. Optimum Boiler Pressure Drop Coefficient Versus Work/Heat Ratio







Figure 5.7. Equipment Cost Versus Work/Heat Ratio

## 5.3 <u>Comparison with Alternative and the Selection</u> of Overall Optimum

The alternative to a cogeneration system is typically taken as a low pressure boiler or furnace, and purchasing electricity from the utility. It is when the economics of the optimally designed cogeneration system are compared to the alternative, that a system's true potential can be shown.

The amortized capital cost attributable to the low pressure furnace is estimated using the relation

$$Z_{f} = CRF * 153.964 * 10^{0.89476} \log HP$$
 (5.1)

where the boiler horsepower is given by

HP = 33500 \* Q[Q] = [Btu/Hr]

Fixed charges for the low pressure furnace  $(FC_f)$ , are estimated in the same manner as the cogeneration system, at one and a half times the equipment cost. The fuel cost of producing hot water,  $CFuel_f$ , is estimated using the unit cost of fuel, CF, the heat input to the water, Q, and the estimated furnace efficiency

$$CFUEL_{f} = \frac{CF*Q}{\eta_{f}}$$
(5.2)

where the furnace efficiency,  $n_f$ , is taken to be 0.80.
The total cost of producing the hot water by the low pressure furnace,  $\text{CTOT}_{f}$ , is estimated by

$$CTOT_{f} = CFUEL_{f} + FC_{f} + Z_{f}$$
(5.3)

Following the logic of the by-product work method (30), the hot water (steam) produced from a cogeneration system is charged with CTOT<sub>f</sub>, the cost of producing hot water from a low pressure boiler. The balance of the cost of the cogeneration system is then attributable to the shaft work (or electricity) produced. The cost per unit of electricity produced, CE, can be calculated as the difference of the total cost of the cogeneration system and the cost allocated to the hot water, all divided by the amount of electricity produced,

$$CE = \frac{ZTOT + FC - ZTOT_{f}}{E}$$
(5.4)

where

$$E = WA * \eta_g$$
(5.5)

and the generator efficiency,  $n_g$ , is assumed to be ninety-five percent.

In order to select the electricity production which maximizes the profit returned from its sale, the market

price of electricity, MPE, must be known. The net revenue generated by the sale of the cogenerated electricity, NRG, is then expressed

$$NRG = (MPE-CE) *E$$
(5.6)

For a particular hot water requirement the optimal work output will correspond to the point where net revenue generated is a maximum. Figures 5.8-5.10 illustrate net revenue versus the work/heat ratio for a required hot water temperature of 250°F and for various market conditions.

Examination of these curves shows an increase in the optimal amount of electricity as the market price of electricity increases. Also, as fuel costs rise, the optimal amount of electricity production decreases.

## 5.4 <u>Recommendation Concerning the Optimization</u> of a Cogeneration System

In order to evaluate the shadow and marginal prices, numerical derivatives of some constraints were taken. The numerical derivatives were taken with respect to either a pressure, temperature, or enthalpy. The increments used were one psia, one degree Fahrenheit, and one  $Btu/lb_m^{\circ}F$ . Although no problems were encountered using only right handed derivatives, it is suggested that both right and left handed derivatives be taken and the average taken. Care must be taken that the increment chosen does not evaluate the function



Figure 5.8. Net Revenue Generated Versus Work/Heat Ratio for a Fuel Cost of \$2/106 Btu



Figure 5.9. Net Revenue Generated Versus Work/Heat Ratio for a Fuel Cost of \$3/10<sup>6</sup> Btu



-

Figure 5.10. Net Revenue Generated Versus Work/Heat Ratio for a Fuel Cost of \$4/106 Btu

in different regions of the steam tables. Taking both right and left handed derivatives and checking the magnitude of each for large discrepancies should prevent this problem.

Using the computer to evaluate numerical derivatives would be much simpler than obtaining analytical expressions for the various partial derivatives of the costing and constraint equations. This is especially true when these equations are very complicated. Since only the value of the derivative is needed, it is recommended that numerical derivatives be used for complicated functions. It may even be desirable to use only numerical derivatives. In this case, it is suggested that a function subroutine be made for each constraint and the subroutine which evaluates the derivatives call the function subroutines to supply values for the constraints at each point x and then at  $x+\Delta x$  or  $x-\Delta x$ .

In order to use this method, there must be some increment,  $\Delta y_k$ , by which the decision variables change for each iteration. Picking a small increment means the program may have to iterate many times before reaching the optimum; on the other hand, too large an increment may cause the solution to oscillate. In order to solve this problem, the program incorporates two different sets of increment sizes, one set is used when the design is far from the optimum, the other set is used when the design is relatively close. For future work, it is desirable to develop a scheme for altering the magnitude of the increment,  $\Delta y_k$ , based on the magnitude of the dimensionless marginal price,  $\Theta_k$ .

The dimensionless marginal prices defined by Eq. 3.26 put these derivatives on an equivalent basis. The magnitude of these dimensionless prices more accurately reflects the magnitude of the economic benefit which can be realized by changing a decision variable than do the dimensional marginal prices,  $\Theta_{\rm b}$ .

Because of the adaptability of this method to numerical techniques, it is possible to use cost data in various forms. It is possible to use a matrix full of data points and to interpolate between these points. This eliminates the need of having purely analytical costing equations.

The introduction of numerical methods into the optimization scheme has significantly broadened the applicability and ease with which this method may be used. But with any optimization method, the time and money spent must be justified. A direct search of the design space is the simplest optimization method. If such a method were applied to this system, there would be five dependent variables to search, plus the work/heat ratio at various market conditions for a specified hot water temperature. This method has therefore eliminated the random searching of a six dimensional space (five decision variables and total cost) necessary for each set of market conditions (fuel and electricity costs) for each required hot water temperature.

The method presented here is seemingly by far the most desirable of the mature optimization methods studied(41). Its matrix notation and adaptability to numerical methods are well-suited for a computer solution.

Furthermore, this method requires no prior knowledge about the economic value of the interconnecting streams nor about the commodity of value being transferred. The Second Law quantities such as available energy and negentropy need not be introduced into the optimization directly although their effects are evaluated (indirectly) by the shadow and marginal prices. Furthermore, any required Second Law based prices can be obtained by using Eq. 3.24 and 3.25 or using a thermoeconomic accounting technique as described in Reference 30.

There are, however, several drawbacks to this method. The algorithm is that of a highly directed iteration based on the slope of the Lagrangian, evaluated for each generation of decision variables. Therefore, it is possible for the solution to get hung up on a local extremum or saddle point (this is true for many optimization methods). Another minor inconvenience is that the designer must supply a feasible set of decision variables to begin the iteration. However, there is no restriction on this initial set as long as it does not represent an impossible design. With these limitations in mind, this method may be applied to any thermal system.

We recommend this optimization method for application to complex thermal systems. It is recommended that further research and development be pursued to improve this optimization scheme. Such improvements would include

- (1) Development of a scheme which uses the magnitude of the dimensionless marginal prices to select the iteration increments for each decision variable.
- (2) Use of entirely numerical derivatives to evaluate the shadow and marginal prices.
- (3) Use of more intricate cost or costing equations.
- (4) Application of this method to a much more complicated system.

### REVIEW OF BUDGET

Table 6.1 lists the proposed budget and the actual budget. The variations between budgets were due to the following:

- One graduate research assistant was hired for Summer 1982 in order to expedite the loading and debugging of SOLTES.
- This amount of money was needed for operating supplies and expenses.
- No publication fees were required during the grant period. This money was used for operating supplies and expenses.
- 4. No money was needed for the purchase of computer codes. Furthermore, this and nearly half of the original budget for computer time were used to support one graduate research assistant (see item l above).
- No travel expenses were encumbered during the grant period. This money was transferred to operating supplies and expenses.

TABLE 6.1

		Proposed	Actual
Α.	Salaries & Wages		
	<pre>1. Principal Investigator, W. J. Wepfer Academic yr, 1981-82, 1/4 time Summer, 1982, 1/3 time</pre>	6,325 3,800	6,325 3,816
	2. Graduate Research Assistant <sup>1</sup>	0	1,668
	Total, Salaries & Wages	10,125	11,809
Β.	Indirect Costs, 73% of A-1	7,391	7,403
C.	Fringe Benefits, 11.11% of A-1	1,125	1,127
D.	Operating Supplies and Expenses <sup>2</sup>	0	1,173
E.	Publication Fees <sup>3</sup>	500	0
F.	Computer Expenses <sup>4</sup>		
	<ol> <li>Computer time</li> <li>Purchase of Codes</li> </ol>	2,000 775	1,068
	Total Computer	2,775	1,068
G.	Travel Expenses <sup>5</sup>	600	0
H.	Total	22,516	22,580
I.	Georgia Tech Contribution (B+C)	8,516	8,580
J.	Engineering Foundation Contribution (H-I)	14,000	14,000

#### 7. PUBLICATIONS AND PRESENTATIONS

The research results, of the present grant period on the development of thermoeconomic modelling, will be submitted for publication:

- Moore, B. B., Wepfer, W. J., "Application of Law Based Design Optimization to Mass Transfer Processes," submitted for publication in the forthcoming American Chemical Society Symposium Series on Second Law Analysis.
- 2. Garceau, R. M., Wepfer, W. J., "Optimization of a Rankine Cycle Cogeneration System," in preparation and to be submitted for publication in the forthcoming American Chemical Society Symposium Series on Second Law Analysis.

APPENDICES

į.

## APPENDIX A

# COMPUTER PROGRAMS GETZ AND LOOKUP FOR THERMODYNAMIC PROPERTY EVALUATION

C, setz SUBROUTINE GETZ(Z, TR, PR, W) С С SUBROUTINE GETZ , GIVEN INPUTS OF REDUCED PRESSURE PR , REDUCED С TEMPERATURE TR AND ACCENTRIC FACTOR W RETURNS THE CORRESPONDING С VALUE OF THE COMPRESSIBILITY FACTOR Z , AS CALCULATED USING THE С METHOD OF PITZER, LIPPMANN, ET AL AS IN "THERMODYNAMICS" BY С PITZER AND BREWER , AS REVISED BY LEWIS AND RANDALL. С REAL PR , TR , W , Z REAL TRMIN , TRMAX , T2MIN , T2MAX , TCMIN , TCMAX REAL PRMIN , PRMAX , P2MIN , P2MAX , PCMIN , PCMAX С PARAMETER (TRMIN=0.80 , TRMAX=4.0) PARAMETER (PRMIN=0.20 , PRMAX=9.0) PARAMETER (T2MIN=0.90 , T2MAX=1.05) PARAMETER (P2MIN=0.40 , P2MAX=1.00) PARAMETER (TCMIN=0.98 , TCMAX=1.15) PARAMETER (PCMIN=1.0 , PCMAX=2.0) С C THE TABLES TO BE USED DEPEND UPON THE INPUT VALUES OF PR AND TR. C IF 0.90 < TR < 1.05 AND 0.40 < PR < 1.00 , THEN THE TABLES FOR C ZO AND Z1 NEAR THE TWO-PHASE REGION SHOULD BE USED. SIMILARLY , C IF 0.92 < TR < 1.15 AND 1.0 < PR < 2.0 , THEN THE TABLES FOR THE AREA NEAR THE CRITICAL REGION SHOULD BE USED. OTHERWISE , THE C C MAIN TABLES SHOULD BE USED UNLESS , OF COURSE , ONE OR BOTH OF THE C INPUT VALUES ARE OFF THE TABLE. IF AN INPUT IS OFF THE TABLE , C A VALUE OF ZERO FOR Z WILL BE RETURNED. IT IS UP TO THE C USER OF THIS ROUTINE TO INTERPRET THIS 'ERROR MESSAGE'. C IF (TR.LT.TRMIN.DR.TR.GT.TRMAX.DR. PR.LT. PRMIN.OR. PR.GT. PRMAX) THEN \$ Z0=0.0 Z1=0.0 ELSE IF (TR.GE.T2MIN.AND.TR.LE.T2MAX.AND. \$ PR.GE.P2MIN.AND.PR.LE.P2MAX) THEN OPEN(7,FILE='FZ02PH',ACCESS='DIRECT',FORM='FORMATTED' ,RECL=G) \$ CALL LOOKUP(TR, PR, ZO) CLOSE(7) DPEN(7,FILE='FZ12PH',ACCESS='DIRECT',FORM='FORMATTED' ,RECL=G) \$ CALL LOOKUP(TR, PR, Z1) CLOSE(7) ELSE IF (TR.GE.TCMIN.AND.TR.LE.TCMAX.AND. PR.GE.PCMIN.AND.PR.LE.PCMAX) THEN \$ OPEN(7,FILE='FZOCRIT',ACCESS='DIRECT',FORM='FORMATTED' \$ ,RECL=G) CALL LOOKUP(TR, PR, ZO) CLOSE(7) OPEN(7,FILE='FZ1CRIT', ACCESS='DIRECT', FORM='FORMATTED'

```
$
         ,RECL=6)
     CALL LOOKUP(TR, PR, Z1)
     CLOSE(7)
  ELSE
     OPEN(7,FILE='FZOMAIN', ACCESS='DIRECT', FORM='FORMATTED'
         ,RECL=G)
 $
     CALL LOOKUP(TR, PR, ZO)
     CLOSE(7)
    OPEN(7,FILE='FZ1MAIN', ACCESS='DIRECT', FORM='FORMATTED'
        ,RECL=G)
$
    CALL LOOKUP(TR, PR, Z1)
   CLOSE(7)
END IF
Z = ZO + (W * Z1)
RETURN
END
```

C, LOOKUP SUBROUTINE LOOKUP(TR, PR, TABVL) C C SUBROUTINE LOOKUP , GIVEN INPUTS OF TR AND PR , RETURNS THE TABLE VALUE FOR THOSE INPUTS FROM THE TABLE DATA FILE THAT IS CURRENTLY C С OPEN. AN UNDERSTANDING С OF THE FILE STRUCTURE USED FOR THE TABLE FILES IS С ESSENTIAL IF THIS PROGRAM IS TO BE UNDERSTOOD. BASICALLY , C THE TABLE FILES ARE FORMATTED , DIRECT ACCESS FILES. С THE FIRST RECORD IN THE FILE CONTAINS A NUMBER THAT CORRESPONDS С TO THE NUMBER OF COLUMNS IN THE TABLE. RECORD TWO IS THE NUMBER С OF ROWS IN THE TABLE. RECORDS 2+1 TO 2+COLS HOLD REAL VALUED С COLUMN HEADINGS , WITH 2+1 HOLDING THE LEFTMOST COLUMN HEADING C AND 2+COLS HOLDING THE RIGHTMOST. SIMILARLY , RECORDS 2+COLS+1 С THROUGH 2+COLS+ROWS HOLD REAL VALUED ROW HEADINGS , IN ORDER С FROM TOP TO BOTTOM. RECORDS 2+COLS+ROWS+1 THROUGH 2+COLS+ROWS+COLS С HOLD THE FIRST ROW OF TABULAR DATA. RECORDS 2+COLS+ROWS+COLS+1 С THROUGH 2+COLS+ROWS+COLS+COLS HOLDS THE SECOND ROW OF TABULAR С DATA. RECORDS 2+COLS+ROWS+(N-1)\*COLS+1 THROUGH 2+COLS+ROWS+ С (N-1)\*COLS+COLS HOLD THE NTH ROW OF DATA. A MORE DETAILED C EXPLAINATION OF THIS SCHEME CAN BE FOUND IN THE EXTERNAL С DOCUMENTATION. C C REAL TR, PR, TABVL, COLIND(30), ROWIND(30), TABVL1, TABVL2 REAL PRIND(2), TRIND(2), TABVLS(2,2) INTEGER I, CREC, COLS, ROWS, IPRIND(2), ITRIND(2) C C FILL COLUMN AND ROW INDEX ARRAYS READ(7, '(F6.3)', REC=1) X COLS=IFIX(X) READ(7, '(F6.3)', REC=2) X ROWS=IFIX(X) DO 100 I = 1 , COLS CREC=2+I 100 READ(7, '(F6.3)', REC=CREC) COLIND(I) DO 120 I = 1 , ROWS CREC=2+COLS+I 120 READ(7, '(F6.3)', REC=CREC) ROWIND(I) C С FIND AND STORE IN PRIND(1) AND PRIND(2) THE VALUES OF THE TWO TABLE COLUMN C HEADINGS THAT PR FALLS BETWEEN. ALSO STIRE THE CORRESPONDING INTEGER C INDICES IPRIND(1) AND IPRIND(2) OBTAINED BY COUNTING FROM LEFT TO C RIGHT ON THE COLUMN HEADINGS UNTIL THE APPRPRIATE COLUMN HEADINGS C ARE REACHED. DO ESSENTIALLY THE SAME THING FOR TR , TRIND'S AND C ITRIND'S , EXCEPT COUNT FROM TOP TO BOTTOM. IF A PR OR TR INPUT C HITS A ROW OR COLUMN HEADING ON THE NOSE , STORE THAT SAME HEADING C AND CORRESPONDING INTEGER INDEX TWICE. C C FIRST , WE'LL DO THE PRIND'S C

```
C
      I = 1
140
      CONTINUE
      IPLUS1=I+1
      IF (PR.EQ.COLIND(I)) THEN
         IPRIND(1)=I
         IPRIND(2) = I
         PRIND(1)=COLIND(I)
         PRIND(2)=COLIND(I)
      ELSE IF (PR.GT.COLIND(I).AND.PR.LT.COLIND(IPLUS1)) THEN
         IPRIND(1) = I
         IPRIND(2) = I + 1
         PRIND(1)=COLIND(I)
         PRIND(2)=COLIND(IPLUS1)
      ELSE
         I = I + 1
         GO TO 140
      END IF
С
 NOW WE'LL DO THE TRIND'S.
С
С
      I=1
160
      CONTINUE
      IPLUS1=I+1
      IF (TR.EQ.ROWIND(I)) THEN
         ITRIND(1) = I
         ITRIND(2) = I
         TRIND(1)=ROWIND(I)
         TRIND(2)=ROWIND(I)
      ELSE IF (TR.GT.ROWIND(I).AND.TR.LT.ROWIND(IPLUS1)) THEN
         ITRIND(1)=I
         ITRIND(2) = I + 1
         TRIND(1)=ROWIND(I)
         TRIND(2)=ROWIND(IPLUS1)
      ELSE
         I = I + 1
         GO TO 160
      END IF
C
С
  WITH THESE INTEGER TABLE INDICES , ACQUIRE APPROPRIATE Z VALUES
С
    FROM THE TABLES
С
С
                                   PR
               1
                   PRIND(1) !
                                          .
                                               PRIND(2)
                                                           [
С
                   IPRIND(1) !
               1
                                           1
                                               IPRIND(2)
                                                           1
С
          -----
                                        _____
С
                  TABVLS(1,1) !
                                           1
                                              TABVLS(1,2)
     TRIND(1) !
                                                            I
1111
    ITRIND(1) !
                              i
                                          1
     _____
              ____
                             ----
C
       TR
             . !
                              1
                                  TABVL !
С
               1
                                           1
C
     _____
C
     TRIND(2) ! TABVLS(2,1) !
                                             TABVLS(2,2)
                                          !
                                                           1
C
    ITRIND(2) !
                             1
                                          1
С
С
С
```

```
С
      CREC=2+ROWS+COLS+(ITRIND(1)-1)*COLS+IPRIND(1)
      READ(7, '(F6.3)', REC=CREC) TABVLS(1,1)
С
      CREC=2+ROWS+COLS+(ITRIND(1)-1)*COLS+IPRIND(2)
      READ(7, '(F6.3)', REC=CREC) TABVLS(1,2)
С
      CREC=2+ROWS+COLS+(ITRIND(2)-1)*COLS+IPRIND(1)
      READ(7, '(F6.3)', REC=CREC) TABVLS(2,1)
С
      CREC=2+ROWS+COLS+(ITRIND(2)-1)*COLS+IPRIND(2)
      READ(7, '(F6.3)', REC=CREC) TABVLS(2,2)
С
С
 INTERPOLATE IN THE APPROPRIATE MANNER
2
    NO INTERPOLATION IS NECESSARY IF TR AND PR BOTH HIT HEADINGS ON THE
С
    NOSE. IF TR ALONE HITS A HEADING ON THE NOSE , DO THE INTERPOLATION
20
    ONE WAY. IF PR ALONE HITS A HEADING ON THE NOSE , DO THE INTERPOL-
    ATION ANOTHER WAY. FINALLY , IF NEITHER PR NOR TR HIT A HEADING ON THE
С
    NOSE , DO A FULL 4-WAY INTERPOLATION.
С
С
      IF (TRIND(1).EQ.TRIND(2)) THEN
         IF (PRIND(1).EQ.PRIND(2)) THEN
            TABVL=TABVLS(1,1)
         ELSE
            TABVL=(PR-PRIND(1))/(PRIND(2)-PRIND(1))*
     $
               (TABVLS(1,2)-TABVLS(1,1))+TABVLS(1,1)
         END IF
      ELSE IF (PRIND(1).EQ.PRIND(2)) THEN
         TABVL=(TR-TRIND(1))/(TRIND(2)-TRIND(1))*
             (TABVLS(2,1)-TABVLS(1,1))+TABVLS(1,1)
     $
      ELSE
         Z1 = (PR - PRIND(1)) / (PRIND(2) - PRIND(1)) *
            (TABVLS(1,2)-TABVLS(1,1))+TABVLS(1,1)
     $
         ZZ=(PR-PRIND(1))/(PRIND(2)-PRIND(1))*
            (TABVLS(2,2) - TABVLS(2,1)) + TABVLS(2,1)
     $
      TABUL=(TR-TRIND(1))/(TRIND(2)-TRIND(1))*(Z2-Z1)+Z1
      END IF
      RETURN
      END
EOI. O FILES. 1 RECS. 635 WORDS.
```

## APPENDIX B

# COMPUTER CODES FOR OPTIMAL DESIGN OF A BINARY SEPARATION SYSTEM

## COMPUTER CODE FOR TRADITIONAL OPTIMIZATION

#### Packed Tower Optimization

This distillation tower is designed to handle 700 lb/mol of feed per hour. The unit is to operate continuously at a total pressure of one atmosphere for 8500 hours per year. The feed contains 45 mol percent benzene and 55 percent toluene. The feed is saturated at its boiling temperature of 201 F.

The Objective:

 Determine the optimum reflux ratio as moles of liquid returned to the tower per mole of distillate product withdrawn.

2) The ratio of the optimum reflux ratio to the minimum reflux ratio.

3) The percent of the total variable cost due to steam consumption at the optimum conditions.

The following conditions apply:

relative volatility equals 2.50

molal heat capacity of liquid mixture is 40 btu/1bmol constant molal heat of vaporization of mixture is 13700 but/1bmol effects of temperature and pressure changes throughout the column is negligible overall coefficient of heat transfer is 80 btu/hr(sq.ft.)F for the reboiler overall coefficient of heat transfer is 100 btu/hr(sq ft )F for the condenser temperature difference driving force in condenser is 50F saturated steam at 60 psia is used in the reboiler temperature of condensing steam is 292.7°F heat of condensation is 915.5 Btu/1b

#### Variable Dictionary

Variable	Description	Units
alpha	relative volatility	none
annbol	annualized boiler cost	\$/yr
anncon	annualized condenser cost	\$/yr
anntow	annualized tower cost	\$/yr.
bolcos	total boiler capital cost	\$
concos	total condenser capital cost	\$
bott	flow rate of bottom product	lbmol/hr
dist	flow rate of overhead prod.	1bmo1/hr
intcpt	intercept of enriching line	none
liq	flow rate of tower fluid	1bmo1/hr
pakcos	packing cost	\$
opstem	operating cost due to steam	\$
opwat	operating cost due to water	\$
vcheck	equilibrium comp. at feed inlet	

ylim enriching line lower composition cannot exceed ycheck zfeed feed composition of most volatile component benzene

PROGRAM TOPT (INPUT, OUTPUT, TAPE5=INPUT, TAPE6=OUTPUT) REAL LIQ,NTU,INTCPT COMMON/STOR1/ DIST,YBOUT,ALPHA,YLIM,XBOT,LIQ,VAP,FEED

SET INITIAL VALUES

YBIN=0.05

YBOUT=0.92

FEED=700.0

ZFEED=0.45

XBOT=YBIN

ALPHA=2.50

DIST=FEED\*(ZFEED-YBIN)/(YBOUT-YBIN)

BOTT=FEED-DIST

DETERMINE TOTAL ANNUAL OPERATING COST FOR DISTILLATION SCHEME

DO 100 R=1.0,1.3,0.01

LIQ=R\*DIST

VAP=(R+1.0)\*DIST

YCHECK=ALPHA\*ZFEED/(1.0+(ALPHA-1.0)\*ZFEED)

CHECK FOR MINIMUM REFLUX RATIO

ANNUALIZED OPERATING COST FOR COOLING WATER

IF (BOLCOS.EQ.100.0) GO TO 80

BOLCOS=TBCOST (VAP, FEED, BOTT)

CALCULATE TOTAL BOILER CAPITAL COST

IF(CONCOS.EQ.100.0) GO TO 80

CONCOS=TCCOST (VAP)

CALCULATE TOTAL CONDENSER CAPITAL COST

TOWCOS=APKCOS+SCOST

WEIGHT\*\*3.0

SCOST=2.862E+03+3.279\*WEIGHT-0.14414E-03\*WEIGHT\*\*2.0+.276E-08\*

WEIGHT=2.0\*RADIUS(R,DIST)\*HEIGHT\*0.05208\*3.14159\*490.0\*1.12

PAKCOS=38.0\*VOLUME

VOLUME=3.14159\*RADIUS(R,DIST)\*\*2.0\*HEIGHT

HEIGHT=NTU(YBIN,YLIM,YBOUT)\*1.64

CALCULATE TOTAL TOWER COST -- SHELL AND PACKING

GO TO 100

PRINT\*,' BELOW MINIMUM REFLUX RATIO'

IF(YLIM.LT.YCHECK) GO TO 50

YLIM=SLOPE\*ZFEED+INTCPT

INTCOP=DIST\*YBOUT/VAP

SLOPE=LIQ/VAP

OPWAT=VAP\*13700.0\*0.054/10000.0\*8500.0/1.0/50.0

#### ANNUALIZED OPERATING COST FOR STEAM

QR=VAP\*13700.0+BOIT\*(227.0-179.0)\*40.0-FEED\*(201.0-179.0)\*40.0 OPSTEM=QR\*0.75/1000.0/915.5\*8500.0

ANNUALIZE CAPITAL COSTS-TAKEN TO BE 15 PERCENT OF TOTAL

ANNTOW=TOWCOS\*0.24

ANNCON=CONCOS\*0.24

ANNBOL=BOLCOS\*0.24

TOTAL ANNUAL VARIABLE COST

TOTCOS=ANNTOW+ANNCON+ANNBOL+OPWAT+OPSTEM

PRINT\*,' REFLUX RATIO EQUALS ',R' TOTAL COST EQUALS ',TOTCOS GO TO 100 PRINT\*,' BEYOND SCOPE OF COST DATA'

CONTINUE

END

This function calculates total condenser cost by interpolating between data taken from Peters & Timmerhaus for condenser cost versus area. The area is calculated by multiplying the vapor flow rate by the heat of vaporization of the mixture and then dividing by the overall heat transfer coefficient and the temperature driving force of the cooling water.

#### FUNCTION TCCOST (VAP)

REAL AREA(4),CCOND(4),DIFF(4) DATA AREA /800.0,1000.0,1200.0,1400.0/ DATA CCOND /9750.0,11250.0,12600.0,13800.0/ DATA DIFF /7.5,6.75,6.0,5125/ TCCOST=100.0 COUNT=0.0

A=VAP\*13700.0/100.0/89.0 IF (A.GT.1600.0) GO TO 20 DO 10 I=4,1,-1 IF (A.GT.AREA(I)) COUNT=I CONTINUE IF (COUNT.LT.1) GO TO 20 TCCOST=CCOND(COUNT) + (A-AREA(COUNT))\*DIFF(COUNT) RETURN END

> The algorithm here is identical to the previous function except that the heat transfer needed is calculated differently. See Peters and Timmerhouse example on tower optimization.

```
FUNCTION TBCOST(VAP,FEED,BOTT)
REAL AREA(4),CBOIL(4),DIFF(4)
DATA AREA /1000.0,1400.0,1800.0,2200/
```

DATA CBOIL /17250.0,21150.0,24600.0,27750.0/ DATA DIFF /9.75,8.625,7.875,6.375/ TBCOST=100.0 COUNT=0.0

QR=VAP\*13700.0+BOTT\*(227.0-179.0)\*40.0-FEED\*(201.0-179.0)\*40.0 A=QR/80.0/(292.7-227) IF(A.GT.2600.0) GO TO 20 DO 10 I=4,1,-1 IF(A.GT.AREA(I)) COUNT=I CONTINUE IF(COUNT.LT.1) GO TO 20 TBCOST=CBOIL(COUNT) +(A-AREA(COUNT))\*DIFF(COUNT) RETURN

END

This function calculates the required number of mass transfer units required for the desired separation. The tower is divided into two distinct sections: the stripping section and the enriching section. There also are two different operating lines associated with each section. This function also uses an integrating routine called \*integ\* to perform the integration. The limits of integration on the stripping section are ybin which is the entering or bottom composition of Benzene and ylim which is the intersection of the two operating lines. Similarly the limits of integration on the enriching section are ylim and ybout which is the product composition of Benzene.

FUNCTION NTU (YBIN, YLIM, YBOUT)

EXTERNAL INTEG,AUX REAL NTU, INTEG,NTUB,NTUT NTUB=INTEG(AUX,YBIN,YLIM) NTUT-INTEG(AUX,YLIM,YBOUT) NTU-NTUB+NTUT RETURN END

This subroutine is used by inte to obtain the integrating function (in this case 1/(ybe-yb)). Note that it must distinguish between stripping and enriching operating lines.

```
SUBROUTINE AUX(Y,FY)
COMMON /STOR1/ DIST,YBOUT,ALPHA,YLIM,XBOT,LIQ,VAP,FEED
REAL LIQ,INTCPT,LPRIM
IF(Y.GT.YLIM) THEN
SLOPE=LIQ/VAP
INTCPT=DIST*YBOUT/VAP
ELSE
```

```
INTCPT= -XBOT* (FEED-DIST)/VAP
LPRIM=LIQ+FEED
SLOPE=LPRIM/VAP
END IF
X= (Y-INTCPT)/SLOPE
YBE=ALPHA*X/(1.0+(ALPHA-1.0)*X)
FY=1.0/(YBE-Y)
RETURN
END
```

This function calculates an integral between the limits a,b and over the function returned by subroutine aux. It uses a gaussian quadrature integrating scheme outlined in a text by Carnahan, Luther, and Wilkes on Numerical Methods.

```
FUNCTION INTEG(AUX,A,B)
```

REAL A, B, FX, INTEG

DIMENSION Z(8), WEIGHT(8)

DATA Z /0.0 ,0.2011940939,0.3941513470,

0.5709721726,0.7244044313,0.8482065834,

0.9372733924,0.9879925180/

DATA WEIGHT /0.2024782419,0.1984314853,

0.1861610001,0.1662692058,0.1395706779,

0.1071592204,0.0703660474,0.0307532419/

124

C=(B-A)/2.0D=(B+A)/2.0SUM=0.0 DO 5 J=1,8 CALL AUX(-Z(J)\*C+D,FX)F3=FX CALL AUX (D, FX) F1=FX CALL AUX (Z(J)\*C+D,FX)F2=FX IF(Z(J).EQ.0.00) SUM=SUM+WEIGHT(J)\*F1 IF (Z(J).NE.0.0) SUM=SUM+WEIGHT (J)\*F2+F3) CONTINUE INTEG=C\*SUM RETURN END

> This function subprogram calculates the operating diameter of a packed tower based on the method presented in Peters & Timmerhaus, page 762 thru 764.

### FUNCTION RADIUS(R,DIST)

REAL MUL, LIQ

Variable such as operating pressure and temperature must be initialized. The data for viscosity and density was acquired from Perry and Chilton and taken to be an average value over the range of variation.

RHOG=0.2 RHOL=50.0 MUL=0.5 PF=150 PRESS=1.0 TEMP=639.0

> Calculation of vapor and liquid molar flow rates are based on simple mass balance taken at the top of the tower

VAP=(R+1.0)\*DIST

LIQ=R\*DIST

X=LIQ/VAP\*SQRT(RHOG/RHOL)

IF(X.LT.0.6) THEN

FX=0.2146446-0.731135\*X+0.831209\*X\*\*2.0-0.3138423\*X\*\*3.0

+0.2761848\*X\*\*4.0

ELSE IF (X.GT.0.6.AND.X.LT.0.8) THEN

FX=1

ELSE

FX=0.0337619=0.015142857\*X+0.001380925\*X\*\*2.0 END IF VALLOW=0.6\*SQRT(FX\*32.17\*RHOL)/(PF\*RHOL\*MUL\*\*0.2)) ACSECT=VAP\*0.73\*TEMP/(PRESS\*VALLOW)/3600.0 RADIUS=0.5\*SQRT(4.0\*ACSECT/3.14159) END

## COMPUTER CODE FOR SECOND LAW METHOD

## <u>Second Law Analysis</u> of a Binary Distillation System

This computer code is designed to calculate the various flows of available energy and entropy penalty function in a simple binary distillation network. The unit cost of product is determined based on the minimum work of separation and is printed out along with other values which can be found in Table

#### Variable Dictionary

Variable	Description	Units
Anntow	annualized tower costs	\$/yr
Aux	subroutine used by Intes	
Intex	integrating subroutine which uses a Gaussian	
	Quadrature integration scheme	
Pfunct	entropy penalty function supplied to the system	
Pfunctl	entropy penalty function used by the tower	
Parcos	the costs associated with the use of available	
	energy and entropy penalty functions	
Tstow	the available energy consumed by the tower	

PROGRAM NEWOPT (INPUT, OUTPUT, TAPE5=INPUT, TAPE6=OUTPUT)

#### REAL LIQ, NTU, INTCPT, MDOT

COMMON/STOR1/ DIST, YBOUT, ALPHA, YLIM, XBOT, LIQ, VAP, FEED

#### SET INITIAL VALUES

YBIN=0.05

YBOUT=0.92

FEED=700.0

ZFEED=0.45

XBOT=YBIN

WORKM=337684.0

ALPHA=2.50

DIST=FEED\*(ZFEED-YBIN)/(YBOUT-YBIN)

BOTT=FEED-DIST

#### DETERMINE TOTAL ANNUAL OPERATING COST FOR DISTILLATION SCHEME

DO 100 R=1.0,1.4,0.01

LIQ=R\*DIST

VAP=(R+1.0)\*DIST

YCHECK=ALPHA\*FEED/(1.0+(ALPHA-1.0)\*ZFEED)

#### CHECK FOR MINIMUM REFLUX RATIO

SLOPE=LIQ/VAP

INTCPT=DIST\*YBOUT/VAP

YLIM=SLOPE\*ZFEED+INTCPT

IF (YLIM.LT.YCHECK) GO TO 50 PRINT\*,' BELOW MINIMUM REFLUX RATIO' GO TO 100

CALCULATE TOTAL TOWER COST -- SHELL AND PACKING

HEIGHT=NTU(YBIN,YLIM,YBOUT)\*1.64

VOLUME=3.14159\*RADIUS(R,DIST)\*\*2.0\*HEIGHT

DIAM=2.0\*RADIUS(R,DIST)

PAKCOS=38.0\*VOLUME

WEIGHT=2.0\*RADIUS(R,DIST)\*HEIGHT\*0.052508\*3.14159\*490.0\*1.12

SCOST=2.862E+03+3.279\*WEIGHT-0.14414E-03\*WEIGHT\*\*2.0+.276E-08\*

WEIGHT\*\*3.0

TOWCOS=PAKCOS+SCOST

Q=VAP\*13700.0

QR=VAP\*13700.0+BOTT\*(227.0-179.0)\*40.0-FEED\*(201.0-179.0)\*40.0

ABOIL=QR/80.0/(292.7-227)

MDOT=Q/50.0

TSTOW=TSDOT(YBIN,YLIM,YBOUT,VAP)

TSCOND=MDOT\*550.0\*0.008764 PFUNCT=Q-TSCOND-MDOT\*2.14

PFUNCT1=PFUNCT-550.0\*QR/687.0

2.5

PARCOS=14.69E-06\* (TSTOW+WORKM)+2.58E-06\*PFUNCT1

#### ANNUALIZE CAPITAL COSTS-TAKEN TO BE 15% OF TOTAL

ANNTOW=TOWCOS\*0.24

TOTAL ANNUAL VARIABLE COST

TOTCOS=(PARCOS+ANNTOW/8500.0)/WORKM

PRINT\*,'',R,' ',HEIGHT,' ',DIAM,' ',TSTOW,' ',PFUNCT1,

', ANNTOW, '', TOTCOS

PRINT\*

GO TO 100

PRINT\*,' BEYOND SCOPE OF COST DATA'

CONTINUE

END

FUNCTION NTU (YBIN,YLIM,YBOUT) EXTERNAL INTEG,AUX REAL NTU,INTEG,NTUB,NTUT NTUB=INTEG (AUX,YBIN,YLIM) NTUT=INTEG (AUX,YLIM,YBOUT) NTU=NTUB+NTUT RETURN END
SUBROUTINE AUX(Y,FY)

COMMON /STOR1/ DIST, YBOUT, ALPHA, YLIM, XBOT, LIQ, VAP, FEED

REAL LIQ, INTCPT, LPRIM

IF (Y.GT.YLIM) THEN

SLOPE=LIQ/VAP

```
INTCPT=DIST*YBOUT/VAP
```

ELSE

INTCPT= -XBOT\*(FEED-DIST)/VAP

LPRIM=LIQ+FEED

SLOPE=LPRIM/VAP

END IF

X=(Y-INTCPT)/SLOPE

YBE=ALPHA\*X/(1.0+(ALPHA-1.0)\*X)

FY=1.0/(YBE-Y)

RETURN

END

FUNCTION INTEG(AUX, A, B)

REAL A, B, FX, INTEG

DIMENSION Z(8), WEIGHT(8)

DATA Z /0.0 ,0.2011940939,0.3941513470,

0.5709721726,0.7244044313,0.842065834,

0.9372733924,0.9879925180/

DATA WEIGHT /0.2024782419,0.1984314853,

0.1861610001,0.1662692058,0.1395706779,

0.1071592204,0.0703660474,0.0307532419/

C=(B-A)/2.0

D=(B+A)/2.0

SUM=0.0

DO 5 J=1,8

CALL AUX (-Z(J)\*C+D,FX)

F3=FX

CALL AUX(D,FX)

F1=FX

CALL AUX(Z(J)\*C+D,FX)

F2=FX

IF (Z(J).EQ.0.00) SUM=SUM+WEIGHT (J)\*F1

IF (Z(J).NE.0.0) SUM=SUM+WEIGHT (J)\* (F2+F3)

CONTINUE

INTEG=C\*SUM

RETURN

END

THIS FUNCTION SUBPROGRAM CALCULATES THE OPERATING DIAMETER OF A PACKED TOWER BASED ON THE METHOD PRESENTED IN PETERS & TIMMERHOUSE PAGE 762 THRU 764

FUNCTION RADIUS(R,DIST)

REAL MUL, LIQ

VARIABLE SUCH AS OPERATING PRESSURE AND TEMPERATURE MUST BE INITIALIZED. THE DATA FOR VISCOSITY AND DENSITY WAS ACQUIRED FROM PERRY AND CHILTON AND TAKEN TO BE AN AVERAGE VALUE OVER THE RANGE OF VARIATION.

RHOG=0.2

RHOL=50.0

MUL=0.5

PF=150

PRESS=1.0

TEMP=639.0

CALCULATION OF VAPOR AND LIQUID MOLAR FLOW RATES ARE BASED ON SIMPLE MASS BALANCE TAKEN AT THE TOP OF THE TOWER

VAP=(R+1.0)\*DIST

LIQ=R\*DIST

X=LIQ/VAP\*SQRT(RHOG/RHOL)

IF(X.LT.0.6) THEN

FX=0.2146446-0.731135\*X+0.831209\*X\*\*2.0-0.3138423\*X\*\*3.0

+0.2761848\*X\*\*4.0

ELSE IF (X.GT.0.6.AND.X.LT.0.8) THEN

FX=1

ELSE

FX=0.0337619-0.015142857\*X+0.001380925\*X\*\*2.0

END IF

VALLOW=0.6\*SQRT((FX\*32.17\*RHOL)/(PF\*RHOG\*MUL\*\*0.2)) ACSECT=VAP\*0.73\*TEMP/(PRESS\*YALLOW)/3600.0 RADIUS=0.5\*SQRT(4.0\*ACSECT/3.14159) END

FUNCTION TSDOT (YBIN, YLIM, YBOUT, VAP) EXTERNAL INTEG, AUX2 REAL SDOT, INTEG, SDOTB, SDOTT SDOTB=INTEG(AUX2,YBIN,YLIM) DOTT=INTEG(AUX2,YLIM,YBOUT) TSDOT=(SDOTB+SDOTT)\*YAP\*1.986\*550.0 RETURN

END

ELSE

END IF

SUBROUTINE AUX2(Y,FY)

COMMON /STOR1/ DIST, YBOUT, ALPHA, YLIM, XBOT, LIQ, VAP, FEED REAL LIQ, INTCPT, LPRIM IF (Y.GT.YLIM) THEN

INTCPT=DIST\*YBOUT/VAP

INTCPT= -XBOT\* (FEED-DIST) /VAP

SLOPE=LIQ/VAP

LPRIM=LIQ+FEED

SLOPE=LPRIM/VAP

X=(Y-INTCPT)/SLOPE YBE=ALPHA\*X/(1.0+(ALPHA-1.0)\*X) FY=ALOG(YBE\*(1.0-Y)/Y/(1.0-YBE)) RETURN

END

### COMPUTER CODE FOR REBOILER DESIGN

## Optimization of Two Phase, Two Stream Heat Exchangers

This program varies the inlet steam temperature to find the optimum heat exchanger design based on heat transfer area and available energy consumption. The various enthalpy and entropy values were obtained from a separate reference found in the M.E. Computer Library labeled Steam.

#### Variable Dictionary

Variable	Description	Units	
Al	net available energy supplied to the		
	distillation tower	Btu/hr	
Ast	the net available energy delivered		
	by the steam to the reboiler	Btu/hr	
Hin	the enthalpy of the entering steam	Btu/1bmass	
Sin	the entropy in the entering steam	Btu/lbmass F	
Zdot	amortized capital cost of the		
	reboiler	\$/yr	

PROGRAM MINBOIL (INPUT, OUTPUT, TAPE5=INPUT, TAPE6=OUTPUT) REAL LPRIME, LMIN, MDOT QDOT=9810298.85

TL=687.0

LMIN=0.0

C1=1.374

C2=1.27E+06

DO 50 TH=780.0,700.0,-1.0

T2=TH-460.0

HIN=HGT(T2)

HOUT=HFT(T2)

SIN=SGT(T2)

SOUT=SFT(T2)

MDOT=QDOT/(HIN-HOUT)

AST=MDOT\*(HIN-HOUT-550.0\*(SIN-SOUT)

SCOST=AST\*3.04E-06

SDOT=QDOT\*(TH-TL)/TH/TL

Al=AST-550.0\*SDOT

ZDOT=TBCOST(708.4,,700.0,378.0,TH,TL)\*0.24/8500.0

LPRIME=(SCOST+ZDOT+C1)/(A1-C2)

PRINT\*,' ',T2,' ',SCOST,' ',AST,' ',A1,' ',ZDOT,' ',LPRIME

PRINT\*

IF(LMIN.EQ.0.0) GO TO 30

IF(LPRIME.GT.LMIN) GO TO 50

LMIN=LPRIME

TMIN=T2

CONTINUE PRINT\* PRINT\*,' INLET STEAM TEMPERATURE EQUALS ',TMIN PRINT\*,' MINIMUM COST OF EXIT AVAILABILITY EQUALS ',LMIN END

FUNCTION TBCOST (VAP, FEED, BOTT, TH, TL)

REAL AREA(4), CBOIL(4), DIFF(4)

DATA AREA /1000.0,1400.0,1800.0,2200/

DATA CBOIL /17250.0,21150.0,24600.0,27750.0/

DATA DIFF /9.75,8.625,7.875,6.375/

TBCOST=100.0

COUNT=0.0

QR=VAP\*13700.0+BOTT\*(227.0-179.0)\*40.0-FEED\*(201.0-179.0)\*40.0 A=QR/80.0/(TH-TL) IF(A.GT.2600.0) TBCOST=6.375\*A+11175.0 IF(A.GT.2600.0) GO TO 20 DO 10 I=1,4 IF(A.GT.AREA(I)) COUNT=I CONTINUE

IF(A.LT.1000.0) TBCOST=9.75\*A+7500.0

TBCOST=CBOIL(COUNT) + (A-AREA(COUNT))\*DIFF(COUNT)

RETURN

END

# COMPUTER CODE FOR CONDENSER DESIGN

PROGRAM NEGMIN (INPUT, OUTPUT, TAPE5=INPUT, TAPE6=OUTPUT) REAL MDOT, LMT, LAMBDA, LAMNEG, LAMMIN

VAP=2.2\*321.0

Q=VAP\*13700.0

T1=550.0

LAMBDA=13.69E-06

LAMMIN=0.0

DO 50 T2=560.0,635.0,1.0

C=5.4E-06/550.0/ALOG(T2/TL)

LMT = (T2 - T1) / ALOG((639.0 - T1) / (639.0 - T2))

ACOND=Q/100.0/LMT

MDOT=Q/(T2-T1)

ZDOT=TCCOST(VAP,ACOND)\*0.24/8500.0

EDOT=MDOT\*T1\*(T2/T1-1.0-ALOG(T2/T1))

SDOT=MDOT\*(ALOG(T2/T1)-(T2-T1)/639.0)

EDOTRJ=Q-EDOT

LAMNEG=(ZDOT+LAMBDA\*(EDOT+550.0\*SDOT)+C\*EDOTRJ)/

(EDOTRJ-550.0\*SDOT)

PRINT\*,' ',T2,' ',MDOT,' ',ZDOT,' ',LAMNEG

IF (LAMMIN.EQ.0.0) GO TO 30 IF (LAMNEG.GT.LAMMIN) GO TO 50 LAMMIN=LAMNEG TMIN=T2 PRINT\*

CONTINUE

PRINT\*,' MINIMUM COST OF NEGENTROPY IS ',LAMMIN PRINT\*,' OPTIMUM DISCHARGE TEMPERATURE ',TMIN END

FUNCTION TCCOST (VAP, ACOND) REAL AREA(4), CCOND(4), DIFF(4) DATA AREA /800.0,1000.0,1200.0,1400.0/ DATA CCOND /9750.0,11250.0,12600.0,13800.0/ DATA DIFF /7.5,6.75,6.0,5.25/ TCCOST=100.0 COUNT=0.0

A=ACOND

IF (A.GT.1600.0) TCCOST=5.25\*A+6450.0 IF (A.GT.1600.0) GO TO 20 DO 10 I=1,4 IF (A.GT.AREA(I)) COUNT=1 CONTINUE IF(COUNT.LT.1) GO TO 20

TCCOST=CCOND(COUNT) + (A-AREA(COUNT))\*DIFF(COUNT)

RETURN

END

#### APPENDIX C

#### THE LAGRANGE METHOD OF UNDETERMINED MULTIPLIERS

In many optimization problems situations occur in which the function to be extremized, the objective function, depends on variables which are not all independent, but are interrelated by equations of constraint. The general situation is to maximize or minimize the objective function, subject to certain constraints.

Objective function 
$$\phi_0 = \phi_0(\{x_i\}, \{y_k\})$$
 (C.1)

Constraints 
$$\phi_{j} = \phi_{j}(\{x_{i}\}, \{y_{k}\}) \quad j = 1, n$$
 (C.2)

where  $\{y_k\}$  is a set of independent variables which represent the number of degrees of freedom in the problem and  $\{x_i\}$  is the set of dependent variables. Given n+m variables and n constraint equations, it follows that there are m independent variables and n dependent variables.

One obvious method of solution is to substitute the constraint equations into the objective function thus eliminating the dependent variables. However, for problems containing a large number of variables, this approach is an algebraic nightmare. To avoid this problem, one can use the

Lagrange Method of Undetermined Multipliers, in which certain unknown multipliers are introduced into the problem. Although Lagrange's method increases the number of variables, it nevertheless simplifies the solution of systems of algebraic equations and is particularly well suited to many engineering optimization problems.

A function, L, called the Lagrangian is defined as

$$L = \phi_{0} + \sum_{j} \lambda_{j} \phi_{j}$$
 (C.3)

where each Lagrangian Multiplier,  $\lambda_j$ , is associated with the constraint equation,  $\phi_j$ . The Lagrangian multipliers are functions of the dependent and independent variables.

$$\lambda_{j} = \lambda_{j}(\{x_{i}\}, \{y_{k}\})$$
 (C.4)

These Lagrangian multipliers may be interpreted as prices associated with a differential change in the corresponding dependent variables.

The Lagrangian is made independent of the dependent variables,  $\{x_i\}$ , by differentiating the Lagrangian with respect to each  $x_i$  and setting each partial derivative of L equal to zero.

$$\frac{\partial \mathbf{L}}{\partial \mathbf{x}_{i}} = \frac{\partial \phi_{0}}{\partial \mathbf{x}_{i}} + \sum_{j} \lambda_{j} \frac{\partial \phi_{j}}{\partial \mathbf{x}_{i}} + \sum_{j} \phi_{j} \frac{\partial \lambda_{j}}{\partial \mathbf{x}_{i}} = 0 \quad i = 1, n \quad (C.5)$$

As long as the set of constraints are arranged in the form  $\phi_{i} = 0$ , the last term in Eq.C.5 is zero so that

$$\frac{\partial L}{\partial x_{i}} = \left(\frac{\partial \phi_{0}}{\partial x_{i}}\right) + \sum_{j} \lambda_{j} \frac{\partial \phi_{j}}{\partial x_{i}} = 0 \quad i = 1, n \quad (C.6)$$

This yields a set of linear equations in the unknown Lagrangian multipliers,  $\{\lambda_j\}$ . This set of equations may be solved yielding Lagrangian multipliers,  $\{\lambda_j\}$ , defined in such a way that the Lagrangian, L, is guaranteed to be independent of the set of dependent variables,  $\{x_i\}$ , and is said to be unconstrained.

The first derivative of the Lagrangian, L, with respect to the set of independent variables,  $\{y_k\}$ , (provided the set  $\{\phi_j = 0\}$  is satisfied) is the derivative of the objective function,  $\phi_0$ , and may be used to locate the coordinates of the extremum. This may be expressed as

$$\frac{\partial L}{\partial y_k} = \frac{\partial \phi_0}{\partial y_k} + \sum_j \lambda_j \frac{\partial \phi_j}{\partial y_k} = \theta_k \qquad k = 1, m \qquad (C.7)$$

where  $\theta_k = 0$  at the extremum.

# APPENDIX D

# LAGRANGE'S METHOD USING JACOBIANS

Lagrange method of undetermined multipliers requires taking partial derivatives of the constraint equations and objective function with respect to the state and decision variables. It is often convenient to use matrix notation to describe these equations.

Lagrange's method requires that these two sets of equations must be solved.

$$\frac{\partial \mathbf{L}}{\partial \mathbf{x}_{i}} = \frac{\partial \phi_{0}}{\partial \mathbf{x}_{i}} + \sum_{j=1}^{n} \lambda_{j} \frac{\partial \phi_{j}}{\partial \mathbf{x}_{i}} = 0 \quad i = 1, n \quad (D.1)$$

$$\frac{\partial L}{\partial y_k} = \frac{\partial \phi_0}{\partial y_k} + \sum_{j=1}^n \lambda_j \frac{\partial \phi_j}{\partial y_k} = \theta_k \quad k = 1, k \quad (D.2)$$

Equation D.1 will generate n simultaneous equations which are linear in the unknown Lagrangian multipliers. Putting this in matrix form yields

$$\begin{bmatrix} \frac{\partial \phi_{0}}{\partial \mathbf{x}_{i}} \end{bmatrix} + \begin{bmatrix} \lambda_{j} \end{bmatrix} \begin{bmatrix} \frac{\partial \phi_{j}}{\partial \mathbf{x}_{i}} \end{bmatrix} = 0$$
 (D.3)

where

$$\begin{bmatrix} \partial \phi \\ 0 \end{bmatrix}$$
 is a l by n matrix (D.3a)

$$[\lambda_{i}]$$
 is a 1 by n matrix (D.3b)

$$\begin{bmatrix} \frac{\partial \phi}{\partial x_{i}} \end{bmatrix}$$
 is a n by n matrix (D.3c)

Rearranging Eq. D.3 yields

$$[\lambda_{j}] \begin{bmatrix} \frac{\partial \phi_{j}}{\partial x_{i}} \end{bmatrix} = - \begin{bmatrix} \frac{\partial \phi_{o}}{\partial x_{i}} \end{bmatrix}$$
(D.4)

Because this equation is of the form  $A\bar{X} = B$ , Cramers rule may be applied directly for the  $\lambda_j$ 

$$[\lambda_{j}] = - \left[\frac{\partial \phi_{o}}{\partial x_{i}}\right] \left[\frac{\partial \phi_{j}}{\partial \phi x_{i}}\right]^{-1}$$
 (D.5)

Each Lagrangian multiplier,  $\lambda_j$ , may now be expressed as the ratio of two determinants, each containing derivatives of the constraint equations and objective function. These determinants, called Jacobians, are of the form

$$D = \begin{vmatrix} \frac{\partial \phi_1}{\partial x_1} & \frac{\partial \phi_2}{\partial x_1} & \frac{\partial \phi_3}{\partial x_1} & \cdots & \frac{\partial \phi_n}{\partial x_1} \\ \frac{\partial \phi_1}{\partial x_2} & \frac{\partial \phi_2}{\partial x_2} & \frac{\partial \phi_3}{\partial x_2} & \cdots & \frac{\partial \phi_n}{\partial x_2} \\ \frac{\partial \phi_1}{\partial x_3} & \frac{\partial \phi_2}{\partial x_3} & \frac{\partial \phi_3}{\partial x_3} & \cdots & \frac{\partial \phi_n}{\partial x_3} \\ \vdots & & & & \\ \frac{\partial \phi_1}{\partial x_n} & \frac{\partial \phi_2}{\partial x_n} & \frac{\partial \phi_3}{\partial x_n} & \cdots & \frac{\partial \phi_n}{\partial x_n} \end{vmatrix}$$

$$(D.6)$$

where the determinant D is written using the notation

$$D = J \left[ \frac{\phi_1, \phi_2, \phi_3, \dots, \phi_n}{x_1, x_2, x_3, \dots, x_n} \right]$$
(D.7)

In terms of Jacobians then, the j-th shadow price,  $\boldsymbol{\lambda}_{j},$  is written

$$\lambda_{j} = \frac{-J\left[\frac{\phi_{1}, \phi_{2}, \dots, \phi_{j-1}, \phi_{0}, \phi_{j+1}, \dots, \phi_{n}}{x_{1}, x_{2}, \dots, x_{j-1}, x_{j}, x_{j+1}, \dots, x_{n}}\right]}{J\left[\frac{\phi_{1}, \phi_{2}, \dots, \phi_{j-1}, \phi_{j}, \phi_{j+1}, \dots, \phi_{n}}{x_{1}, x_{2}, \dots, x_{j-1}, x_{j}, x_{j+1}, \dots, x_{n}}\right]}$$
(D.8)

$$= -J[A_{j}]/J[B]$$
(D.8a)

A similar manipulation may be performed on Eq.D.2 to put it in matrix form

$$[\theta_{k}] = \left[\frac{\partial \phi_{o}}{\partial y_{k}}\right] + \left[\lambda_{j}\right] \left[\frac{\partial \phi_{j}}{\partial y_{k}}\right]$$
(D.9)

Using the definition of the shadow prices from Eq. 3 8 each marginal price may be expressed

$$\theta_{k} = \frac{\partial \phi_{o}}{\partial y_{k}} - \sum_{j=1}^{n} \left\{ \frac{J[A_{j}]}{J[B]} \frac{\partial \phi_{j}}{\partial x_{j}} \right\}$$
(D.10)

or (since J[B] is a scalar independent of the counter j)

$$\theta_{k} = \frac{\frac{\partial \phi_{o}}{\partial y_{k}} J[B] - \sum_{j=1}^{n} J[A_{j}] \frac{\partial \phi_{j}}{\partial y_{k}}}{J[B]}$$
(D.11)

or

$$\theta_{k} = \frac{J\begin{bmatrix} \frac{\phi_{1}, \phi_{2}, \dots, \phi_{n}}{x_{1}, x_{2}, \dots, x_{n}} \end{bmatrix} \frac{\partial \phi_{0}}{\partial y_{k}} - \sum_{j=1}^{n} J\begin{bmatrix} \frac{\phi_{1}, \phi_{2}, \dots, \phi_{0}, \dots, \phi_{n}}{x_{1}, x_{2}, \dots, x_{j}, \dots, x_{n}} \end{bmatrix} \frac{\partial \phi_{j}}{\partial y_{k}}}{J\begin{bmatrix} \frac{\phi_{1}, \phi_{2}, \dots, \phi_{n}}{x_{1}, x_{2}, \dots, x_{n}} \end{bmatrix}}$$
(D.12)

The numerator of Eq. D.12 is the cofactor of the determinant

$$D = J\left[\frac{\phi_{1}, \phi_{2}, \dots, \phi_{n}, \phi_{0}}{x_{1}, x_{2}, \dots, x_{n}, y_{k}}\right]$$
(D.13)

so that the marginal price may be expressed as the ratio of two determinants

$$\theta_{k} = \frac{J\left[\frac{\phi_{1}, \phi_{2}, \dots, \phi_{n}, \phi_{0}}{x_{1}, x_{2}, \dots, x_{n}, y_{k}}\right]}{J\left[\frac{\phi_{1}, \phi_{2}, \dots, \phi_{n}}{x_{1}, x_{2}, \dots, x_{n}}\right]} = \frac{J\left[C_{k}\right]}{J\left[B\right]}$$
(D.14)

#### APPENDIX E

## DERIVATION OF SHADOW AND MARGINAL PRICE EQUATIONS

State Variables

Decision Variables

$$\{y_k\} = \{AN, DN, P1, P2, AR\}$$

#### Solving for the Shadow Prices {SP(i)}

Equations 3.10 are used to solve for the shadow prices. The matrix interpretation of this equation is found in Table 4.4. Using this matrix as a guide the blocks which are zero are easily identified. This is done by checking the functional dependence of each constraint and of the objective function. The derivatives which need to be evaluated may be done explicitly without use of the chain rule. The computation of A,Athe non-zero elements in Table 4.4 is presented below.

$$SP(16) = \frac{\partial}{\partial CA}(ZC)$$

$$CA \leq 3000$$

$$SP(16) = X31*FCR*FCPW*FCP*FCB*\frac{\partial}{\partial CA} (FCA1)$$

$$\frac{\partial}{\partial CA} [FCA1] = \frac{\partial}{\partial CA} [CA*C31*EXP(B31*ALOG CA)$$

$$\frac{\partial}{\partial CA} [FCA1] = CA*C31*EXP(B31*ALOG CA)*B31*\frac{1}{CA} + C31*EXP(B31*ALOG CA)$$

$$SP(16) = X31*FCR*FCPW*FCB*FCP*C31EXP(B31*ALOG CA)*(B31+1)$$

$$SP(16) = (ZC/CA)*(B31+1)$$
(E.1)

$$CA > 3000$$
  

$$SP(16) = X31*FCR*FCPW*FCP*FCB*\frac{\partial}{\partial CA} (FCA2)$$
  

$$\partial/\partial CA(FCA2) = \frac{\partial}{\partial CA} (CA*C36) = C36$$
  

$$SP(16) = X31*FCR*FCPW*FCP*C36$$
  

$$SP(16) = (ZC/CA) (E.1b)$$

$$SP(15) = \frac{\partial}{\partial TM} [SP(16)*\phi 16] = \frac{\partial}{\partial TM} [SP(16)*HWM*CPW* (TB-TC)/(TM*U)]$$
  
= -SP(16)\*HWM\*CPW\*(TB-TC)/(U\*TM\*\*2)  
$$SP(15) = -SP(16)*CA/TM (E.2)$$

$$SP(14) = \frac{\partial}{\partial T3} [SP(15)*_{\phi}15] = [\frac{\partial}{\partial T3} [{(T3-TC)-(T2-TB)}] / ALOG[(T3-TC)/(T2-TB)]]*SP(15)$$

 $SP(14) = SP(15)*{ALOG[(T3-TC)/(T2-TB)]*1-[(T3-TC)-(T2-TB)]*}$   $\{1/(T2-TB)\}*[(T2-TB)/(T3-TC)]*1\}/{ALOG[(T3-TC)/(T2-TB)]**2}$   $SP(14) = SP(15)*{ALOG[(T3-TC)-(T2-TB)]-[1-(T2-TB)/(T3-TC)]}/$   $\{ALOG[(T3-TC)/(T2-TB)]\}**2$ 

$$SP(11) = \frac{\partial}{\partial H2S} (SP(12)*_{\phi}12) = SP(12)*_{\frac{\partial}{\partial H2S}}[(WA+WP)/((H1-H2S)*STM) = SP(12)*(WA+WP)/(((H1-H2S)**2)*STM)*(-1)*(-1)$$

$$SP(11) = SP(12)*BN/(H1-H2S)$$
(E.6)

$$SP(11) = \frac{\partial}{\partial H2S} (SP(12)*_{\phi}12) = SP(12)*\frac{\partial}{\partial H2S} [(WA+WP)/((H1-H2S)*STM)]$$
  
= SP(12)\*(WA+WP)/(((H1-H2S)\*\*2)\*STM)\*(-1)\*(-1)

$$SP(11) = \frac{\partial}{\partial H2S} (SP(12)*_{\phi}12) = SP(12)*_{\frac{\partial}{\partial H2S}}[(WA+WP)/((H1-H2S)*STM)]$$
  
= SP(12)\*(WA+WP)/(((H1-H2S)\*\*2)\*STM)\*(-1)\*(-1)

$$SP(12) = X21*FBT*FBW[FBN*B21/BN+(FBN-1)*B24/(1-BN)]$$
 (E.5)

= FBW\*B21/BN

$$= B24*[(1-BNS)/(1-BN)]**B24$$
 (1-BN)

$$- B0/2[(1 BNG)/(1 CN)] + + C0/((1 CN))$$

$$= [(1-BNS)**B24]*[(1-BN)**(-B24-1)*(-1)]*B24(-1)$$

$$\frac{\partial}{\partial BN}$$
 (FBN) =  $\frac{\partial}{\partial BN}$  (1+[(1-BNS)/(1-BN)]\*\*B24)

$$\frac{\partial}{\partial BN} (FBW) = \frac{\partial}{\partial BN} [EXP(B21*ALOG[B22*BN*STM*(F2T+F2P)])]$$
$$= FBW*B21*\{1/B22*BN*STM*(F2T+F2P\}*B22*STM + (F2T+F2P)\}$$

$$SP(12) = \frac{\partial}{\partial BN} [ZB] = X21 * FBT * \frac{\partial}{\partial BN} [FBW * FBN]$$
$$\frac{\partial}{\partial BN} [FBW * FBN] = FBN * \frac{\partial}{\partial BN} (FBW) + FBW + \frac{\partial}{\partial BN} (FBN)$$

$$SP(13) = \frac{\partial}{\partial HF} [CF*HF] = CF$$
 (E.4)

$$/ \{ALOG[(T3-TC)/(T2-TB)]\}**2$$
 (E-3)

$$SP(14) = SP(15) * \{ALOG[(T3-TC)/(T2-TB)] - 1 + (T2-TB)/(T3-TC)]\}$$

$$\begin{split} & \text{SP}(10) = \frac{\partial}{\partial T1} [\text{SP}(11) *_{\phi} 11 + 2\text{A} + 2\text{B}] \\ & \frac{\partial}{\partial T1} \phi 11 = (\text{H2S}(\text{P1}, \text{P2}, \text{T1} + \text{DT1}) - \text{H2S}(\text{P1}, \text{P2}, \text{T1})) / \text{DT1} = \text{DER1} \\ & \frac{\partial}{\partial T1} (\text{ZA}) = \text{X11*FAP*FAM*FAN*FAR*} \frac{\partial}{\partial T1} \text{FAT} \\ & \frac{\partial}{\partial T1} (\text{ZA}) = \text{X11*FAP*FAM*FAN*FAR*} \frac{\partial}{\partial T1} \text{FAT} \\ & \frac{\partial}{\partial T1} (\text{FAT} = \frac{\partial}{\partial T1} (1 + \text{C12*EXP}[(\text{T1} - \text{T1S}) / \text{B13}]) \\ & = (\text{FAT} - 1) / \text{B13} \\ & \frac{\partial}{\partial T1} (\text{ZB}) = \text{X21*FBN*} \frac{\partial}{\partial T1} [\text{FBT*FBW}] \\ & \frac{\partial}{\partial T1} [\text{FBT*FBW}] = \text{FBW*} \frac{\partial}{\partial T1} (\text{FBT}) + \text{FBT*} \frac{\partial}{\partial T1} (\text{FBW}) \\ & \frac{\partial}{\partial T1} (\text{FBT}) = \frac{\partial}{\partial T1} (1 + \text{C22EXP}[(\text{T1} - \text{T1S}) / \text{B23}]) \\ & = (\text{FBT} - 1) / \text{B23} \\ & \frac{\partial}{\partial T1} (\text{FBW}) = \frac{\partial}{\partial T1} (\text{EXP}[\text{B21*ALOG}[\text{FB1*}[\text{CPS*}(\text{T1R} - \text{T2R} - \text{T2R*ALOG}(\text{T1R} / \text{T2R}) + \text{F2P}]]]) \\ & = \text{FBW*}[\text{B21}/(\text{FB1*}(\text{F2T} + \text{F2P}))] * \text{FB1*}\text{CPS}(1 - \text{T2R*}(\frac{\text{T2R}}{\text{T1R}}) * (\frac{1}{\text{T2R}})) \\ & = \text{FBW*}\text{B21*}\text{FB1*}\text{CPS*}(1 - \text{T2R} / \text{T1R}) / (\text{F21} + \text{F2P})) \\ & = \text{FBW*}\text{B21*}\text{FB1*}\text{CPS*}(1 - \text{T2R} / \text{T1R}) / (\text{F21} + \text{F2P}) \\ & = \text{FBW*}\text{B21*}\text{CPS*}(1 - \text{T2R} / \text{T1R}) / (\text{F21} + \text{F2P}) \\ & = \text{FBW*}\text{B21*}\text{CPS*}(1 - \text{T2R} / \text{T1R}) / (\text{F21} + \text{F2P}) \\ & = \text{FBW*}\text{B21*}\text{CPS*}(1 - \text{T2R} / \text{T1R}) / (\text{F21} + \text{F2P}) \\ & = \text{FBW*}\text{B21*}\text{CPS*}(1 - \text{T2R} / \text{T1R}) / (\text{F21} + \text{F2P}) \\ & = \text{FBW*}\text{B21*}\text{CPS*}(1 - \text{T2R} / \text{T1R}) / (\text{F21} + \text{F2P}) \\ & \text{SP}(10) = \text{SP}(11) * \text{DER1} + \text{X11*}\text{FAP*}\text{FAN*}\text{FAR*}\text{FAM*}(\text{FAT} - 1) / \text{B13} \\ & + \text{X21*}\text{FBN*}\text{FBW*}[(\text{FBT} - 1) / \text{B23} + \text{FB1} \times \text{CPS} (1 - \text{T2R} / \text{T1R}) / (\text{F21} + \text{F2P}) ] \\ & (E. 7) \\ \\ & \text{SP}(9) = \frac{\partial}{\partial \text{H1}} [\text{SP}(10) * \phi 10 + \text{SP}(12) * \phi 12 + \text{SP}(13) * \phi 13] \\ & \frac{\partial}{\partial \text{H1}} (\phi 10) = (\text{T1}(\text{H1} + \text{DH1}, \text{P1}) - \text{T1}(\text{H1}, \text{P1}) / \text{DH1} = \text{DER2} \\ \end{aligned}$$

 $\frac{\partial}{\partial HI}$  ( $\phi$ 12) =  $\frac{\partial}{\partial HI}$  [(WA+WP)/((H1-H2S)\*STM)]

= -BN/(H1-H2S)

= ((WA+WP)/STM)\*(-1)/(H1-H2S)\*\*2

$$\frac{3}{3H1} (\phi 13) = \frac{3}{3H1} (STM*(H1-H4)/AN) \\ = STM/AN$$

$$SP(9) = SP(10)*DER2-SP(12)*BN/(H1-H2S)+SP(13)*STM/AN$$
(E.8)
$$SP(8) = \frac{3}{3WP} (SP(9)*\phi 9+SP(12)*\phi 12) \\ = SP(9)/STM+SP(12)/(STM(H1-H2S))$$
(E.9)
$$SP(8) = [SP(9)+SP(12)/(H1-H2S)]/STM$$
(E.9)
$$SP(7) = \frac{3}{3STM} [SP(8)*\phi 8+SP(9)*\phi 9+SP(12)*\phi 12+SP(13)*\phi 13+ZA+ZB+ZD]$$

$$\frac{3}{3STM} [\phi 8] = (H4-H3) = WP/STM$$

$$\frac{3}{3STM} [\phi 9] = -(WA+WP)/STM*22 \\ \frac{3}{3STM} [\phi 12] = -(WA+WP)/(STM*2)*(H1-H2S) = -BN/STM$$

$$\frac{3}{3STM} [\phi 13] = (H1-H4)/AN = HF/STM$$

$$\frac{3}{3STM} [A13] = (H1-H4)/AN = HF/STM$$

$$\frac{3}{3STM} [ZA] = X11*FAP*FAT*FAN*FAR*\frac{3}{3STM} (FAM)$$

$$\frac{3}{3STM} [ZB] = X21*FBT*FBN*\frac{3}{3STM} [FBW]$$

$$\frac{3}{3STM} [ZB] = K21*FBT*FBN*\frac{3}{3STM} [FBW]$$

$$\frac{3}{3STM} [ZD] = X41*FDN*\frac{3}{3STM} (FD1)$$

$$\frac{3}{3STM} [ZD] = X41*FDN*\frac{3}{3STM} (FD1)$$

$$\frac{3}{3STM} [FD1] = FD1*[B41/y2]*(Y2/STM)$$

$$= FD1*B41/STM$$
(E.10)

$$\begin{split} & SP(6) = \frac{\partial}{\partial H4} \left[ SP(8) *_{\phi} + SP(13) *_{\phi} + 13 \right] \\ & SP(6) = SP(8) * STM-SP(13) * STM/AN \end{split} (E.11) \\ & SP(5) = \frac{\partial}{\partial P4} \left[ SP(6) *_{\phi} + 2D \right] \\ & = SP(6) * CF1 * V34/DN + X41 * FDN * \frac{\partial}{\partial P4} (FD1) \\ & \frac{\partial}{\partial P4} (FD1) = FD1 * [B41/y2] * B42 * STM * V34/DN \\ & = FD1 * B41/(P4-P3) \end{aligned} (E.12) \\ & SP(5) = SP(6) * CF1 * V34/DN + ZD * B41/(P4-P3) (E.12) \\ & SP(4) = \frac{\partial}{\partial H3} \left[ SP(6) *_{\phi} + SP(7) *_{\phi} + SP(8) *_{\phi} 8 \right] \\ & = SP(6) + SP(7) * [HWM * CPW * (TB - TC) / (CN * (H2 - H3) * *2) * [-1] * [-1] \\ & SP(8) * STM \end{aligned} (E.13) \\ & SP(4) = SP(6) + SP(7) * STM/(H2 - H3) - SP(8) * STM (E.13) \\ & SP(4) = SP(6) + SP(7) * STM/(H2 - H3) - SP(8) * STM (E.13) \\ & SP(3) = \frac{\partial}{\partial P3} \left[ SP(4) *_{\phi} + SP(6) *_{\phi} + SP(14) *_{\phi} + 4 + ZC + ZD \right] \\ & \frac{\partial}{\partial P3} \left[ \phi 4 \right] = \left[ H3(P3 + DP3, SAT \cdot L) - H3(P3, SAT \cdot L) \right] / DP3 = DER3 \\ & \frac{\partial}{\partial P3} \left[ \phi 6 \right] = - CF1 * V34/DN \\ & CA < 3000 \text{ sq. ft.} \end{aligned} (CA < 3000 sq. ft. \\ & \frac{\partial}{\partial P3} \left[ FCR \right] = B32 * [P3((1/CR) - 1)/C35] * * [B32 - 1] * (-\frac{1}{CR} - 1)/C35 = B32 * [P3(-1)/CR - 1)/C35] * * B32/P3 \\ & = FCR * B32/P3 \end{aligned}$$

 $\frac{\partial}{\partial P3}$  [ZC] = ZC\*B32/P3

 $SP(2) = SP(15)*[-ALOG(DUM1)+DUM1-1]/{ALOG(DUM1)}**2$ 

+ZB\*B21\*[-CPS\*ALOG(T1R/T2R)+R\*ALOG(P1/P2)]/(F2T+F2P)

$$-ZC*B34/(T2-TB-5)**2$$
(E.15)
$$SP(1) = \frac{\partial}{\partial H2} [SP(7)*\phi7+SP(9)\phi9]$$

 $= SP(7) *HWM+CPW*(TB-TC) / \{CN*(H2-H3)**2\}(-1)+SP(9)$ SP(1) = -SP(7)\*STM/(H2-H3)+SP(9) (E.16)

#### Solving for the Marginal Prices {PM(i)}

Equations 3.13 are used to solve for the shadow prices. The matrix interpretation of this equation is found in Table 4.6. Using this matrix as a guide the blocks which are zero are easily identified. This is done by checking the functional dependence of each constraint and of the objective function. The derivatives which need to be evaluated may be done explicitly without use of the chain rule. The computation of the non-zero elements in Table 4.6 is presented below.

$$PM(1) = \frac{\partial}{\partial AN} [SP(13)*\phi 13+ZA]$$

$$\frac{\partial}{\partial AN} [\phi 13] = -STM*(H1-H4)/AN**2 = -HF/AN$$

$$\frac{\partial}{\partial AN} [ZA] = X11*FAP*FAM*FAT*FAR*\frac{\partial}{\partial AN} (FAN)$$

$$\frac{\partial}{\partial AN} [FAN] = B14*[(1-ANS)/(1-AN)]**(B14-1)*[(1-ANS)/(1-AN)]**(B14-1)*[(1-ANS)/(1-AN)]**2]$$

$$= (FAN-1)*B14/(1-AN)$$

$$PM(1) = -SP(13)*HF/AN+X11*FAP*FAM*FAT*FAR*$$

(FAN-1)\*B14/(1-AN)

(E.17)

$$\begin{split} \mathsf{PM}(2) &= \frac{\partial}{\partial DN} \ [\mathsf{SP}(6) \phi 6 + \mathsf{ZD}] \\ &= -(\mathsf{H4} + \mathsf{H3}) / \mathsf{DN} \ [\mathsf{FD1}] + \mathsf{FD1} \ \frac{\partial}{\partial \mathsf{DN}} \ [\mathsf{FDN}] ] \\ &= -\mathsf{FD1} * [\mathsf{B41} / \mathsf{y2}] * [-\mathsf{y2} / \mathsf{DN}] \\ &= -\mathsf{FD1} * \mathsf{B41} / \mathsf{DN} \\ &= -\mathsf{FD1} * \mathsf{B41} / \mathsf{DN} \\ &= -\mathsf{FD1} * \mathsf{B41} / \mathsf{DN} \\ &= (\mathsf{FDN} - 1) * \mathsf{B43} / (1 - \mathsf{DN}) \ ] * * (\mathsf{B43} - 1) \} * \mathsf{B43} * \frac{1 - \mathsf{DNS}}{(1 - \mathsf{DN}) * * \mathsf{Z}} \\ &= (\mathsf{FDN} - 1) * \mathsf{B43} / (1 - \mathsf{DN}) \\ &= (\mathsf{FDN} - 1) * \mathsf{B43} / (1 - \mathsf{DN}) \end{split} \end{split}$$

$$\begin{aligned} \mathsf{PM}(2) &= -\mathsf{SP}(6) * (\mathsf{H4} + \mathsf{H3}) / \mathsf{DN} + \mathsf{X41} * \mathsf{FD1} * [-\mathsf{FDN} * \mathsf{B41} / \mathsf{DN} + (\mathsf{FDN} - 1) * \mathsf{B43} / (1 - \mathsf{DN})) \end{aligned}$$

$$\begin{aligned} \mathsf{PM}(2) &= -\mathsf{SP}(6) * (\mathsf{H4} - \mathsf{H3}) / \mathsf{DN} + \mathsf{X41} * \mathsf{FD1} * [-\mathsf{FDN} * \mathsf{B41} / \mathsf{DN} + (\mathsf{FDN} - 1) * \mathsf{B43} / (1 - \mathsf{DN})) \end{aligned}$$

$$\begin{aligned} \mathsf{PM}(2) &= -\mathsf{SP}(6) * (\mathsf{H4} - \mathsf{H3}) / \mathsf{DN} + \mathsf{X41} * \mathsf{FD1} * [-\mathsf{FDN} * \mathsf{B41} / \mathsf{DN} + (\mathsf{FDN} - 1) * \mathsf{B43} / (1 - \mathsf{DN})) \end{aligned}$$

$$\begin{aligned} \mathsf{PM}(2) &= -\mathsf{SP}(6) * (\mathsf{H4} - \mathsf{H3}) / \mathsf{DN} + \mathsf{X41} * \mathsf{FD1} * [-\mathsf{FDN} * \mathsf{B41} / \mathsf{DN} + (\mathsf{FDN} - 1) * \mathsf{B43} / (1 - \mathsf{DN})) \end{aligned}$$

$$\begin{aligned} \mathsf{PM}(3) &= \frac{\partial}{\partial \mathsf{PT}} (\mathsf{SP}(5) * \phi 5 + \mathsf{SP}(10) * \phi 10 + \mathsf{SP}(11) * \phi 11 + \mathsf{ZA} + \mathsf{ZB}) \end{aligned}$$

$$\begin{aligned} \frac{\partial}{\partial \mathsf{PT}} [\phi 5] &= 1 / \mathsf{AR} \\ \frac{\partial}{\partial \mathsf{PT}} [\phi 10] &= [\mathsf{T1}(\mathsf{H1}, \mathsf{P1} + \mathsf{DP1}) - \mathsf{T1}(\mathsf{H1}, \mathsf{P1}] / \mathsf{DP1} = \mathsf{DER5} \\ \frac{\partial}{\partial \mathsf{PT}} [\phi 11] &= [\mathsf{H2S}(\mathsf{P1} + \mathsf{P1}, \mathsf{P2}, \mathsf{T1}) - \mathsf{H2S}(\mathsf{P1}, \mathsf{P2}, \mathsf{T1})] / \mathsf{DP1} = \mathsf{DER6} \\ \frac{\partial}{\partial \mathsf{PT}} [\mathsf{ZA}] &= \mathsf{X11} * \mathsf{FAM} * \mathsf{FAT} * \mathsf{FAR} * \mathsf{FAN} * \frac{\partial}{\partial \mathsf{PT}} [\mathsf{FAP}] \\ \frac{\partial}{\partial \mathsf{PT}} [\mathsf{ZA}] &= \mathsf{ZA} * \mathsf{B11} \\ \frac{\partial}{\partial \mathsf{PT}} [\mathsf{ZB}] &= \mathsf{Z2} * \mathsf{B11} \\ \frac{\partial}{\partial \mathsf{PT}} [\mathsf{ZB}] &= \mathsf{Z2} * \mathsf{B21} * \mathsf{R} * \mathsf{T2} \mathsf{R} / [\mathsf{P1} * (\mathsf{F2} \mathsf{T} + \mathsf{F2} \mathsf{P})] \\ \frac{\partial}{\partial \mathsf{PT}} [\mathsf{ZB}] &= \mathsf{ZB} * \mathsf{B21} * \mathsf{R} * \mathsf{T2} \mathsf{R} / [\mathsf{P1} * (\mathsf{F2} \mathsf{T} + \mathsf{F2} \mathsf{P})] \\ \frac{\partial}{\partial \mathsf{PT}} [\mathsf{ZB}] &= \mathsf{ZB} * \mathsf{B21} * \mathsf{R} * \mathsf{T2} \mathsf{R} / [\mathsf{P1} * (\mathsf{F2} \mathsf{T} + \mathsf{F2} \mathsf{P})] \end{aligned}$$

$$PM(3) = SP(5)/AR+SP(10)*DER5+SP(11)*DER6+ZA+B11+ZB*B21*R*T2R/[P1*(F2T*F2P)] (E.19)
$$PM(4) = \frac{\partial}{\partial P2} [SP(1)*\phi1+SP(2)*\phi2+SP(3)*\phi3+SP(11)*\phi11+ZB+ZC]\frac{\partial}{\partial P2} [\phi1] = [H2(P2+DP2,X2)-H2(P2,X2)]/DP2 = DER7\frac{\partial}{\partial P2} [\phi2] = [T2(P2+DP2)-T2(P2)]/DP2 = DER8\frac{\partial}{\partial P2} [\phi3] = CR\frac{\partial}{\partial P2} [\phi3] = CR\frac{\partial}{\partial P2} [zB] = X21*FBT*FBN*\frac{\partial}{\partial P2} [FBW]\frac{\partial}{\partial P2} [ZB] = X21*FBT*FBN*\frac{\partial}{\partial P2} [FBW]\frac{\partial}{\partial P2} [ZB] = SBW*[B21/{FB1*(F2T+F2P)}]*FB1*r*T2R*\frac{P2}{P1}*(-P1/P2**2)= -FBW*B21*R*T2R/(P2*(F2T+F2P))
CA < 3000 sq. ft.\frac{\partial}{\partial P2} [ZC] = X31*FCA1*FCR*FCDW*FCB*\frac{\partial}{\partial P2} [FCP]= X31*FCA1*FCR*FCPW*[C33+2*C34*P2]
CA > 3000 sq. ft.\frac{\partial}{\partial P2} [ZC] = X31+FCA2*FCR*FCPW*FCB*(C33+2*C34*P2]
DUM2 = SP(1)*DER7+SP(2)*DER8+SP(3)*CR+SP(11)*DER9-ZB*B21*R*T2R/(P2*(F2T+F2P))
DUM3 = X31*FCP*FCR*FCPW*FCB*(C33+2*C34*P2)
CA < 3000 sq. ft.PM(4) = DUM2+DUM3*FCA1 (E.20a)
CA > 3000 sq. ft.PM(4) = DUM2+DUM3*FCA2 (E.20b)$$$$

.

$$PM(5) = \frac{\partial}{\partial AR} [SP(5)*\phi5+ZA]$$

$$\frac{\partial}{\partial AR} [\phi5] = -P1/AR**2$$

$$\frac{\partial}{\partial AR} [ZA] = X11*FAP*FAM*FAT*FAN*\frac{\partial}{\partial AR} [FAR]$$

$$\frac{\partial}{\partial AR} [FAR] = \{[(1-ARS)/(1-AR)]**[B15-1]\}*B15*\frac{1-ARS}{(1-AR)**2}$$

$$= B15*(FAR-1)/(1-AR)$$

$$PM(5) = -SP(5)*P1/AR**2+X11*FAP*FAM*FAT*$$

.

$$FAN*(FAR-1)*B15/(1-AR)$$
 (E.21)

/

# APPENDIX F

# COMPUTER PROGRAM USED TO OPTIMIZE THE COGENERATION SYSTEM (INCLUDING SAMPLE OUTPUT)





FROGRAM Z(INFUT,OUTPUT,TAPE5=INPUT,TAFE6=OUTPUT,OUT,TAFE7=OUT) С С C С THIS FROGRAM WAS WRITTEN BY ROBERT M. GARCEAU AS PART C OF THE M. S. THESIS ENTITLED: . С C THERMOECONOMIC OFTIMIZATION OF A RANKINE CYCLE COGENERATION SYSTEM С С C THIS FROGRAM IS DESIGNED TO OPTIMIZE A FOUR COMPONENT C С RANKINE CYCLE COGENERATION SYSTEM. SYSTEM DESCRIPTION: THIS SYSTEM IS DESIGNED SUCH THAT С IT PRODUCES TWO PRODUCTS 1)SHAFT WORK (WHICH MAY BE С. CONVERTED OT ELECTRICTY) AND 2)HOT WATER FROM THE COOLING C WATER SIDE OF THE CONDENSER. C THE FOUR COMPONENTS OF THIS SYSTEM ARE THE A)BOILER С C B) BACK PRESSURE TURBINE/GENERATOR C) COUNTER FLOW CONDENSER C AND D) BOILER FEED PUMP. THE SYSTEM IS ARRANGED SO THAT С THE CONDENSING STEAM SUPPLIES THE NECESSARY ENERGY C TO HEAT THE CONDENSER COOLING WATER TO THE REQUIRED TEMPERATURE. THIS MEANS THE STEAM MUST CONDENSE AT С С A RELATIVELY HIGH PRESSURE. CHANGING THE BASIC С SYSTEM OR THE FORM OF THE COSTING EQUATIONS FOR С THE EQUIPMENT WILL REQUIRE CHANGES THROUGH OUT THE PROGRAM (ALTERING A CONSTRAINT EFFECTS NOT С C ONLY THAT CONSTRAINT BUT ANY SHADOW OR MARGINAL FRICES ASSOCIATED WITH IT). С THIS PROGRAM MAY BE EASILY EDITED TO ALLOW FOR С CHANGES IN THE INFLATION RATE WHICH WILL BE REFLECTED E С BY ALTERING THE CAPITAL RECOVERY FACTOR (CRF), THE С COST OF FUEL, AND/OR THE ASSOCIATED CONSTANTS IN

C CAFITAL COSTING EQUATIONS.

С	IN ORDER	TO OFERATE THIS PROGRAM IT IS NECESSARY	
C	TO SPECIFY T	HE PRODUCT REQUIREMENTS (THE HOT WATER	
C	MASS FLOW RA	TE, INLET AND OUTLET TEMPERATURES, AND	
С	THE SYSTEM N	ET SHAFT WORK OUTPUT). ONCE THE REQUIRED	
С	PRODUCTS ARE	SPECIFIED AN INITIAL DESIGN MUST BE	
C	INFUT. THIS	INITIAL DESIGN DOES NOT HAVE TO BE NEAR	
С	THE OFTIMUM,	IF THE INITIAL DESIGN IS IMPOSSIBLE	
С	FOR THERMODY	NAMIC REASONS THE PROGRAM WILL TELL THE	
С	USER HOW TO	CORRECT THE FRORLEM AND ASK FOR NEW	
С	INFUT PARAME	TERS. EXAMPLE: IF THE SPECIFIED TURBINE	
C	OUTLET FRESS	URE IS TO LOW SUCH THAT ITS TEMPERATURE	
С	IS LOWER THAN	N THE REQUIRED OUTLET TEMPERATURE OF THE	
С	HOT WATER FRI	DM THE CONDENSER, THE PROGRAM WILL RESPOND	
С	"P2 IS TO LOW"		
С	"INFUT HWM, "	TB (HOT), TC, WA"	
С	THEN THE USE	R WILL TRY AGAIN.	
С	******	*******	
С		GLOSSARY OF TERMS	
С	STATE FOINT		
С	1	BOILER OUTLET, TURBINE INLET	
С	2	TURBINE OUTLET, CONDENSER INLET	
С	з	CONDENSER OUTLET, PUMP INLET	
С	4	FUMF OUTLET, BOILER INLET	
С	С	CONDENSER COOLING WATER INLET	
С	в	HOT WATER TO PROCESS	
С	SYMBOL	DEFINITION	
С	A	COMPONENT A IS THE BOILER	
С	AN	BOILER FIRST LAW EFFICIENCY	
Ċ	ANS	REFERENCE BOILER FIRST LAW EFFICIENCY	
С	AR:	BOILER PRESSURE DROP COEFFICIENT	
С	ARS	REFERENCE BOILER PRESSURE DROP COEFFICIENT	
С	B	COMPONENT B IS THE TURBINE	

С	B	CAPITAL COSTING CONSTANT
С	BN	TURBINE ISENTROFIC EFFICIENCY
С	BNS	REFERENCE TURBINE ISENTROPIC EFFICIENCY
С	С	COMPONENT C IS THE CONDENSER
С	C	CAPITAL COSTING CONSTANT
С	CA	CONDENSER HEAT TRANSFER AREA [FT**2]
С	CF	FUEL COST E\$/10**6 BTU]
С	CF1	CONVERSION FACTOR E144PSI/PSFJ/[778.16 FT LB/BTU]
С	CFUEL	TOTAL FUEL COST [\$/HR]
С	CN	CONDENSER FIRST LAW EFFICIENCY
С	CPS	SPECIFIC HEAT OF STEAM [NTU/LB F]
С	CPW	SPECIFIC HEAT OF WATER ERTU/LB FJ
С	D	COMFONENT D IS THE PUMP
С	D	INCREMENT FOR NUMERICAL DERIVATIVE
С	DELAVL	AVAILABLE ENERGY OF HOT WATER TO PROCESS [BTU/HR]
С	DER_	VALUE OF NUMEICAL DERIVATIVE NUMBER _
С	DERIV_	SUBROUTINE WHICH EVALUATES NUMERICAL DERIVATIVE
С		NUMBER _
С	IUMMY_	DUMMY VARIABLE USED TO STORE A VALUE OF A LONG
с		EXFRESSION WHICH IS USED REFEATEDLY
С	ETTA2	SYSTEM SECOND LAW EFFICIENCY (ASSUMING HF=AF)
С	н	ENTHALPY
С	HF	TOTAL HEAT INPUT BY THE FUEL EBTU/HRD
С	P	PRESSUER [PSIA]
с	FM(I)	DIMENSIONLESS MARGINAL PRICE I
С	PURZ_	PURCHASE COST OF COMPONENT _ E\$J
С	PURZSYS	SUM OF ALL COMPONENT PURCHASE COSTS [\$]
С	R	UNIVERSAL GAS CONSTANT EBTU/LB FJ
С	SF(I)	SHADOW PRICE I
С	т	TEMPERATURE [F]
Ċ	T_R	TEMPERATURE [R]
С	тм	LOG MEAN TEMPERATURE DIFFERENCE LF OR RJ
С	U	OVERALL HEAT TRANSFER COEFFICIENT EBTU/LB F FT**2]

С	V43	AVERAGE SPECIFIC VOLUME BETWEEN 3 & 4 [FT**3/LB]		
С	WA	NET TURBINE OUTPUT EBTU/HRJ		
С	WF	WORK INFUT TO PUMP EBTU/HR]		
С	×_	STEAM QUALITY		
С	Z	AMORTIZED CAPITAL COST OF COMPONENT _ [\$/HR]		
С	ZTOLD	AMORTIZED CAPITAL COST OF THE SYSTEM FOR THE PREVIOUS		
С		ITERATION [\$/HR]		
С	ZTOT	SUM OF ALL AMORTIZED COMPONENT CAPITAL COSTS [\$/HR]		
С	****	************		
	COMMON SP(16)	PM(5),F1,P2,F3,P4,PB,PC,T1,T2,T3,TB,TC,T15,DUMMY		
	COMMON T1R, T2F	R;H1;H2;H2S;H3;H4;X2;V34;CPW;CPS;TM;AN;BN;CN;DN;ANS		
	COMMON BNS, DNS	S,ARS,AR,CR,U,R,CRF,DP3,DP1,DP2,DT1,DH1,CF1,WA,WP,CA		
	COMMON HWM,STM	1,C11,C12,B11,B12,B13,B14,B15,X11,FAF,FAM,FAT,FAN,FAR		
	COMMON C21,C22	2,821,822,823,824,X21,F8T,F81,F8N,F2T,F2P,F8W,C31,C32		
	COMMON C33,C34	,C35,C36,B31,B32,B33,X31,FCA1,FCA2,FCR,FCPW,FCP,C41		
	COMMON 841,842	2,843,X41,FDN,FD1,Y2,ZA,ZB,ZC,ZD,CF,HF,ZTOLD,K,COUNT		
	COMMON ZTOT, CF	FUEL,B34,FCB		
40	CALL VALUE			
50	CALL CONSTR			
	WRITE(6,*)T2,8	я		
	IF (T2 .LE. TH	IF (T2 .LE. TB) GO TO 51		
	IF (BN .GE. 1.	O) GO TO 53		
	GO TO 59			
51	CONTINUE			
52	FORMAT("P2 IS	TO LOW">		
	WRITE(6,52)			
	GO TO 40			
53	CONTINUE			
54	FORMAT(*P1 IS	FORMAT("P1 IS TO LOW")		
	WRITE(6,54)			
	GD TD 40			
59	CONTINUE			
	CALL COST			
CFUEL=CF\*HF ZTOT=ZA+ZB+ZC+ZD+CFUEL CALL SHADOW

CALL MARGIN

60 FORMAT(1X,\* ZA=\*,E15.9,\* ZB=\*,E15.9,\* ZC=\*,E15.9,\* ZD=\*,E15.9
!,\* CFUEL=\*,E15.9,\* ZTOT=\*,E15.9)
WRITE(6,60)ZA,ZB,ZC,ZD,CFUEL,ZTOT
COUNT=COUNT+1

IF(COUNT.LE.5)GO TO 120

- 62 FORMAT(1X, \*NEW GENERATION\*) WRITE(6,62)
- 10 FORMAT(1X, "AN=", FB.6, " DN=", FB.6, " P1=", FB.3, " P2=", FB.3
  - !, AR=",F8.6, BN=",F8.6, T1=",F8.3, T2=",F8.3)

WRITE(6,10)AN, DN, F1, F2, AR, BN, T1, T2

DO 75 I=1,5

WRITE(6,\*)I,FM(I)

- 75 CONTINUE
- B0 FORMAT(1X,\*D0 YOU WISH TO ITERATE (ANSWER 1=N0,2=YES)\*)
  WRITE(6,80)
- 100 FORMAT(I1)
  - READ(5,100)IANS

IF(IANS.EQ.1)GO TO 125

DUMMY=ABS(ZTOT-ZTOLD)

ZTOLD=ZTOT

IF(DUMMY.GT.3.0)G0 TO 120

COUNT=1

120 CONTINUE

CALL NEWVAL

GO TO 50

- 125 CONTINUE
- CALL OUTPUT STOP END

SUBROUTINE VALUE

С С

С С THIS SUBROUTINE INITIALIZES ALL ECONOMIC, THERMODYNAMIC AND ALGERBRAIC CONSTANTS. THIS SUBRUOTINE ALSO ACCEPTS THE C INITIAL DESIGN, THE FIRST GENERATION OF DECISION VARIABLES С NECESSARY TO BEGIN THE ITERATION PROCESS. С COMMON SF(16), PM(5), F1, F2, F3, F4, PB, PC, T1, T2, T3, TB, TC, T15, DUMMY COMMON T1R, T2R, H1, H2, H25, H3, H4, X2, V34, CPW, CPS, TM, AN, BN, CN, DN, ANS COMMON BNS, DNS, ARS, AR, CR, U, R, CRF, DP3, DP1, DP2, DT1, DH1, CF1, WA, WF, CA COMMON HWM, STM, C11, C12, B11, B12, B13, B14, B15, X11, FAF, FAM, FAT, FAN, FAR COMMON C21,C22,B21,B22,B23,B24,X21,FBT,FB1,FBN,F2T,F2F,FBW,C31,C32 COMMON C33,C34,C35,C36,E31,E32,E33,X31,FCA1,FCA2,FCR,FCFW,FCP,C41 COMMON B41, B42, B43, X41, FDN, FD1, Y2, ZA, ZB, ZC, ZD, CF, HF, ZTOLD, K, COUNT COMMON ZTOT, CFUEL, B34, FCB CR=0.99 FB=300.0 FC=297.0 CN=1.0 X2=.95 FORMAT(1X, "INPUT HWM, TB(HOT), TC, WA") 5 WRITE(6,5) READ(5,\*)HWM, TB, TC, WA FORMAT(1X, "HWM=", E15.9," TB=", F8.2," TC=", F8.2," WA=", E15.9) 6 WRITE(6,6)HWM, TB, TC, WA FORMAT(1X, "INPUT AN, DN, P1, F2, AR") 10 WRITE(6,10) READ(5,\*)AN, DN, P1, P2, AR 20 FORMAT(1X, "INPUT THE COST OF FUEL \$/MILLION BTU") WRITE(6,20) READ(5,\*)CFBIG CF=CFBIG\*(1E-6)

CRF=1.875E-5 ANS=0.90 ARS=0.92 T1S=1100.0 C11=20.15522241 C12=5.0 B11=1.4110546E-3 B12=.771879549 B13=18.75 B14=7.0 B15=8

С

BNS=0.95 C21=5.240378E+3 C22=5.0 B21=0.56932344 B22=3.929119E-4 B23=18.75 B24=3.0

С

C31=426.2632633 C32=0.93 C33=2.6380952E-4 C34=1.352381E-6 C35=14.696 C36=1.11 B31=-0.45565133 B32=-0.38 B33=-0.11 B34=0.1

С

DNS=0.80 C41=1969.2325

B41=0.4838546 B42=7.2709088E-5 B43=3.0 ZTOLD=0.0 K=0 COUNT=6 R=0.1102109 CPS=0.55 CPW=1.00 CF1=0.1850519 V34=0.018 U=1000.0 DF3=1.0 DF1=1.0 DF2=1.0 DT1=1.0 DH1=1.0 RETURN END SUBROUTINE CONSTR THIS SUBROURINE CALCULATES THE DEPENDENT VARIABLES FOR FOR EACH GENERATION OF DECISION VARIABLES. THESE VALUES WILL REMAIN CONSTANT FOR THE ENTIRE ITERATION, UNTIL THE DECISION VARIABLES ARE CHANGED. COMMON SP(16), PM(5), P1, P2, P3, P4, PB, PC, T1, T2, T3, TB, TC, T1S, DUHMY COMMON T1R, T2R, H1, H2, H2S, H3, H4, X2, V34, CPW, CPS, TM, AN, BN, CN, DN, ANS COMMON BN5.DN5.AR5.AR.CR.U.R.CRF.DP3.DF1.DP2.DT1.DH1.CF1.WA.WF.CA

С

С

С

C C

С

С

С

С

С

COMMON HWM, STM, C11, C12, B11, B12, B13, B14, B15, X11, FAF, FAM, FAT, FAN, FAR COMMON C21, C22, B21, B22, B23, B24, X21, FBT, FB1, FBN, F2T, F2F, FBW, C31, C32 COMMON C33, C34, C35, C36, B31, B32, B33, X31, FCA1, FCA2, FCR, FCFW, FCF, C41 COMMON 841,842,843,X41,FDN,FD1,Y2,ZA,ZB,ZC,ZD,CF,HF,ZTOLD,K,COUNT COMMON ZTOT, CFUEL, B34, FCB CALL SUBH2(P2+X2+H2) T2=TSL(P2) IF (T2 .LE. TB) GO TO 100 P3=P2\*CR H3=HFF(F3) F'4=F'1/AR H4=H3+CF1\*V34\*(F4-F3)/DN STM=HWM\*CPW\*(TB-TC)/(CN\*(H2-H3)) WF=STM\*(H4-H3) H1 = (WA + WP) / STM + H2T1=TFH(P1,H1)

с с

> H2S=ZSDT(P1,F2,T1,ZS1,ZH1,ZT2,ZX1,ZX2,ZV1,ZV2) BN=(WA+WF)/(STM\*(H1-H2S)) HF=STM\*(H1-H4)/AN

С

CALL SUBT3(F3,T3) TM=((T3-TC)-(T2-TB))/(ALOG((T3-TC)/(T2-TB))) CA=HWM\*CFW\*(TB-TC)/(TM\*U)

#### С

T1R=T1+460.0

С

#### C

100 CONTINUE

RETURN

END

С С SUBROUTINE SUBH2(P+X+H) С THIS SUBROUTINE CALCULATES ENTHALPY WITHIN THE TWO С PHASE REGION OF THE STEAM TABLES. С HG=HGF(P) HF=HFP(P) H=HF+X\*(HG-HF) RETURN END С С SUBROUTINE SUBT3(F,T) С С THIS SUBROUTINE CALCULATES THE TEMPERATURE CORRESPONDING С TO A PRESSURE IN THE TWO PHASE REGION OF THE STEAM TABLES. H=HFP(P) T=TSLH(H) RETURN END C С SUBROUTINE COST С THIS SUBROUTINE CALCULATES THE ESTIMATED AMORTIZED CAPITAL С С INVESTMENT FOR EACH GENERATION OF DECISION AND DEPENDENT VARIABLES. COMMON SP(16), PH(5), P1, P2, P3, P4, PB, PC, T1, T2, T3, TB, TC, T1S, DUMMY COMMON T1R, T2R, H1, H2, H2S, H3, H4, X2, V34, CPW, CPS, TM, AN, BN, CN, DN, ANS COMMON BNS, DNS, ARS, AR, CR, U, R, CRF, DP3, DP1, DP2, DT1, DH1, CF1, WA, WF, CA COMMON HWM, STM, C11, C12, B11, B12, B13, B14, B15, X11, FAP, FAM, FAT, FAN, FAR COMMON C21, C22, B21, B22, B23, B24, X21, FB1, FB1, FBN, F2T, F2P, FBW, C31, C32 COMMON C33, C34, C35, C36, B31, B32, B33, X31, FCA1, FCA2, FCR, FCFW, FCF, C41

```
COMMON B41, B42, B43, X41, FDN, FD1, Y2, ZA, ZB, ZC, ZD, CF, HF, ZTOLD, K, COUNT
      COMMON ZTOT, CFUEL, B34, FCB
С
С
           BOILER COST
С
      X11=CRF*C11
      FAF=EXF(B11*F1)
      FAM=EXF(B12*ALOG(STM))
      FAT=1.0+C12*EXF((T1-T15)/B13)
      FAN=1.0+((1.0-AN5)/(1.0-AN))**B14
      FAR=1.0+((1.0-ARS)/(1.0-AR))**B15
С
С
           TURBINE COST
С
      X21=CRF*C21
      FBT=1.0+C22*EXF((T1-T15)/B23)
      FBN=1.0+((1.0-BNS)/(1.0-BN))**B24
      FB1=B22*BN*STM
      F2T=CPS*(T1R-T2R-T2R*ALOG(T1R/T2R))
      F2P=R*T2R*ALOG(P1/P2)
      FBW=EXP(B21*ALOG(FB1*(F2T+F2P)))
С
           CONDENSER COST
С
С
      X31=CRF
      FCB=EXF(B34/(T2-TB-5))
      FCR=(P3*((1.0/CR)-1.0)/C35)**B32
      FCPW=((PC-PB)/C35)**B33
      FCP=C32+C33*P2+C34*(P2**2)
      FCA1=CA*C31*EXP(B31*ALOG(CA))
      FCA2=CA*C36
С
C
           PUMP COST
```

С X41=CRF\*C41 FDN=1.0+((1.0-DNS)/(1.0-DN))\*\*B43 Y2=B42\*STM\*V34\*(P4-P3)/DN FD1=EXP(B41\*ALOG(Y2)) С С COMPUTE ALL AMORTIZED CAPITAL COSTS С ZA=X11\*FAF\*FAM\*FAT\*FAR\*FAN ZB=X21\*FBT\*FBN\*FBW IF (CA.GT.3000.0) GD TO 100 С FOR CA<3000.0 SQ. FT. ZC=X31\*FCA1\*FCF\*FCR\*FCPW\*FCB GO TO 200 С FOR CA>3000 SR. FT. 100 CONTINUE ZC=X31\*FCA2\*FCF\*FCR\*FCFW\*FCB 200 CONTINUE ZD=X41\*FDN\*FD1 С RETURN END С С SUBROUTINE SHADOW С THIS SUBROUTINE CALCULATES THE VALUE FOR THE SHADOW PRICES С ASSOCIATED WITH EACH CONSTRAINT CORRESPONDING TO THE INPUT SET С OF DEPENDENT AND DECISION VARIABLES. THIS SUBROUTINE CALLS С SUBROUTINES DERIV1 THROUGH DERIV4 TO EVALUATE THE NUMERICAL С DERIVATIVES WHICH USE THE LIBRARY SUBROUTINE STEAM. Ć COMMON SP(16), PM(5), P1, P2, P3, P4, PB, PC, T1, T2, T3, TB, TC, T1S, DUMMY COMMON T1R, T2R, H1, H2, H2S, H3, H4, X2, V34, CPW, CPS, TM, AN, BN, CN, DN, ANS COMMON BNS, DNS, ARS, AR, CR, U, R, CRF, DP3, DP1, DP2, DT1, DH1, CF1, WA, WP, CA COMMON HWM, STM, C11, C12, B11, B12, B13, B14, B15, X11, FAP, FAM, FAT, FAN, FAR COMMON C21, C22, B21, B22, B23, B24, X21, FBT, FB1, FBN, F2T, F2F, FBW, C31, C32 COMMON C33, C34, C35, C36, B31, B32, B33, X31, FCA1, FCA2, FCR, FCPW, FCP, C41 COMMON B41, B42, B43, X41, FDN, FD1, Y2, ZA, ZB, ZC, ZD, CF, HF, ZTOLD, K, COUNT COMMON ZTOT, CFUEL, B34, FCB IF (CA.GT.3000.0) GD TO 100 SF(16)=ZC\*(B31+1.0)/CA

GD TO 200

100 CONTINUE

SF(16)=ZC/CA

200 CONTINUE

SP(15)=-SP(16)\*CA/TM

DUM1=((T3-TC)/(T2-TB))

SP(14)=SP(15)\*(ALOG(DUM1)+(1.0/DUM1)-1.0)/(ALOG(DUM1))\*\*2

SF(13)=CF

SF(12)=X21\*FBT\*FBW\*(FBN\*B21/BN+(FBN-1.0)\*B24/(1.0-BN))

SP(11)=SP(12)\*BN/(H1-H2S)

CALL DERIV1(P1,P2,T1,DT1,DER1)

SF(10)=SF(11)\*DER1+X11\*FAP\*FAM\*FAN\*FAR\*(FAT-1.0)/B13+X21\*FBN

!\*FBW\*((FBT-1.0)/B23+FBT\*B21\*CPS\*(1.0-T2R/T1R)/(F2T+F2P))

CALL DERIV2(H1,DH1,P1,DER2)

SP(9)=SP(10)\*DER2+SP(13)\*STM/AN-SP(12)\*BN/(H1+H2S)

SP(8)=SP(9)/STM+SP(12)/(STM\*(H1-H2S))

SF(7)=(SF(8)\*WF-SF(9)\*(WA+WF)/STM-SF(12)\*BN+SF(13)\*HF+

!ZA\*B12+ZB\*B21+ZD\*B41)/STM

SP(6)=SP(8)\*STM-SP(13)\*STM/AN

SP(5)=SP(6)\*CF1\*V34/DN+ZD\*B41/(P4-P3)

SP(4)=SP(6)+SP(7)\*STM/(H2-H3)-SP(8)\*STM

CALL DERIV3(P3,DF3,DER3)

CALL DERIV4(P3,DP3,DER4)

SP(3)=SP(4)\*DER3-SP(6)\*CF1\*V34/DN+SP(14)\*DER4+ZC\*B32

!/F3-ZD#B41/(F4-P3)

```
SP(2)=SP(15)*(-ALOG(DUM1)-1.0+DUM1)/(ALOG(DUM1))**2
     !+ZB*B21*(CPS*(-ALOG(T1R/T2R))+R*ALOG(P1/P2))/(F2T+F2P)
     !-ZC*B34/(T2-TB-5)**2
      SP(1)=-SP(7)*STM/(H2-H3)+SP(9)
      RETURN
      END
С
С
      SUBROUTINE DERIV1(P1,P2,T1,DT1,DER1)
С
      TT1=T1+DT1
      H2S1=ZSDT(F1,F2,T1,S1,H1,T2,X1,X2,V1,V2)
      H2S2=ZSDT(F1,F2,TT1,ZS1,ZH1,ZT2,ZX1,ZX2,ZV1,ZV2)
      DER1=(H2S2-H2S1)/DT1
      RETURN
      END
С
С
      SUBROUTINE DERIV2(H1,DH1,P1,DER2)
С
     TH1=H1+DH1
      T11=TFH(F1+H1)
     T12=TPH(P1,TH1)
     DER2=(T12-T11)/DH1
     RETURN
     END
С
С
     SUBROUTINE DERIV3(P,DP,DER3)
С
     TP=P+DP
.
     H31=HFP(P)
     H32=HFP(TP)
```

DER3=(H32-H31)/DF RETURN END С С SUBROUTINE DERIV4(F,DF,DER4) С TP=P+DP CALL SUBT3(P,T1) CALL SUBT3(TP,T2) DER4=(T2-T1)/DF RETURN END С С SUBROUTINE MARGIN С THIS SUBROUTINE CALCULATES THE VALUE FOR THE DIMENSIONLESS С MARGINAL PRICES, SP(I), CORRESPONDING TO THE INPUT SET OF DECISION С С AND DEFENDENT VARIABLES, AND THE INPUT SET OF SHADOW FRICES. THIS SUBROUTINE CALLS SUBROUTINES DERIV5 THROUGH DERIV9 TO EVALUATE THE С NUMERICAL DERIVATIVES WHICH USE THE LIBRARY SUBROUTINE STEAM. С COMMON SF(16),FM(5),F1,F2,F3,F4,F8,FC,T1,T2,T3,T8,TC,T1S,DUMMY COMMON T1R, T2R, H1, H2, H2S, H3, H4, X2, V34, CPW, CPS, TM, AN, BN, CN, DN, ANS COMMON BNS, DNS, ARS, AR, CR, U, R, CRF, DF3, DF1, DF2, DT1, DH1, CF1, WA, WF, CA COMMON HWM,STM,C11,C12,B11,B12,B13,B14,B15,X11,FAF,FAM,FAT,FAN,FAR COMMON C21, C22, B21, B22, B23, B24, X21, FBT, FB1, FBN, F2T, F2P, FBW, C31, C32 COMMON C33,C34,C35,C36,B31,B32,B33,X31,FCA1,FCA2,FCR,FCPW,FCF,C41 COMMON B41, B42, B43, X41, FDN, FD1, Y2, ZA, ZB, ZC, ZD, CF, HF, ZTOLD, K, COUNT COMMON ZTOT, CFUEL, B34, FCB

Ċ

PM(1)=(-SP(13)\*HF/AN+X11\*FAP\*FAM\*FAT\*FAR\*(FAN-1.0)\*B14/(1.0-AN)) !\*AN/ZTOT

```
PM(2)=(-SP(6)*CF1*V34*(P4-P3)/DN**2+X41*FD1*(B43*(FDN-1.0)
     !/(1.0-DN)-B41*FDN/DN))*DN/ZTDT
      CALL DERIVS(H1,P1,DP1,DER5)
      CALL DERIV6(P1, DF1, P2, T1, DER6)
      PM(3)=(SP(5)/AR+SP(10)*DER5+SP(11)*DER6+ZA*B11+ZB*
     1821*R*T2R/((F2T+F2P)*P1))*P1/ZTOT
      CALL DERIV7(P2,DP2,X2,DER7)
      CALL DERIV8(P2,DP2,DER8)
      CALL DERIV9(P1+P2+DP2+T1+DER9)
      DUM2=SP(1)*DER7+SP(2)*DER8+SP(3)*CR+SP(11)*DER9-ZB*
     1821*R*T2R/(P2*(F2T+F2P))
      DUM3=X31*FCR*FCP*FCPW*(C33+2.0*C34*P2)*FCB
      IF (CA.GT.3000.0) GD TD 100
      PM(4)=(DUM2+DUM3*FCA1)*P2/ZTOT
      GO TO 200
100 CONTINUE
      FM(4)=(DUM2+DUM3*FCA2)*F2/ZTOT
200 CONTINUE
      FM(5)=(-SP(5)*F1/AR**2+X11*FAF*FAM*FAT*FAN*(FAR-1.0)
     1*B15/(1.0-AR))*DN/ZTOT
      RETURN
      END
С
С
      SUBROUTINE DERIV5(H,F,DF,DER5)
С
     TP=P+DP
      T1=TPH(F+H)
      T2=TPH(TF+H)
      DER5=(T2-T1)/DP
      RETURN
      END
C
```

С SUBROUTINE DERIV6(P1,DP1,P2,T1,DER6) С TP=P1+DP1 H1=ZSDT(F1,F2,T1,S,H1,T2,X1,X2,V1,V2) H2=ZSDT(TF,F2,T1,ZS,ZH1,ZT2,ZX1,ZX2,ZV1,ZV2) DER6=(H2-H1)/DF1 RETURN END С С SUBROUTINE DERIV7(P,DP,X,DER7) С TF'=F'+DF'CALL SUBH2(P+X+H1) CALL SUBH2(TP+X+H2) DER7=(H2-H1)/DF RETURN END С С SUBROUTINE DERIV8(P,DP,DER8) С TP=P+DP T21=TSL(F) T22=TSL(TP) DER8=(T22-T21)/DP RETURN END ε С SUBROUTINE DERIV9(P1,P2,DP2,T1,DER9) С

TF2=F2+DF2 H251=ZSDT(F1,F2,T1,S1,H1,T2,X1,X2,V1,V2) H2S2=ZSDT(F1,TF2,T1,S12,H12,T22,X12,X22,V12,V22) DER9=(H2S2-H2S1)/DF2 RETURN END

C C

SUBROUTINE NEWVAL

С

THIS SUBROUTINE SELECTS THE NEW SET OF DECISION VARIABLES С BASED ON THE SIGN OF THE CORRESPONDING DIMENSIONLESS MARGINAL C FRICE, THIS NEW SET OF DECISION VARIABLES IS USED IN THE NEXT C ITERATON. THIS SUBROUTINE OPERATES IN ONE OF TWO MODES. IF C THE MAGNITUDE OF THE FREVIOUS ITERATION'S SYSTEM COST (ZTOLD) C IS DIFFERENT BY AN AMOUNT LARGER THAN SOME PREDETERMINED NUMBER С THAN THE FRESENT ITERATION'S SYSTEM COST THE SUBROUTINE CHANGES C C ALL THE DECISION VARIABLES BASED ON THAT SET OF MARGINAL PRICES. C IF NOT THE SUBROUTINE CHANGES ONLY ONE DECISION VARIABLE AND C REQUIRES A NEW SET OF MARGINAL PRICES TO BE EVALUATED BEFORE

C CHANGING THE NEXT DECISION VARIABLE.

COMMON SF(16), FM(5), P1, F2, F3, P4, FB, PC, T1, T2, T3, TB, TC, T1S, DUMMY COMMON T1R, T2R, H1, H2, H2S, H3, H4, X2, V34, CPW, CFS, TM, AN, BN, CN, DN, ANS COMMON BNS, DNS, ARS, AR, CR, U, R, CRF, DF3, DF1, DF2, DT1, DH1, CF1, WA, WF, CA COMMON HWM, STM, C11, C12, B11, B12, B13, B14, B15, X11, FAF, FAM, FAT, FAN, FAR COMMON C21, C22, B21, B22, B23, B24, X21, FBT, FB1, FBN, F2T, F2P, FBW, C31, C32 COMMON C33, C34, C35, C36, B31, B32, B33, X31, FCA1, FCA2, FCR, FCFW, FCP, C41 COMMON B41, B42, B43, X41, FDN, FD1, Y2, ZA, ZB, ZC, ZD, CF, HF, ZTOLD, K, COUNT COMMON ZTOT, CFUEL, B34, FCB

DIMENSION SIGN(5)

D0 50 J=1,5 SIGN(J)=FM(J)/(ABS(PM(J)))

50 CONTINUE

IF (DUMMY.GT.3.0)GD TD 100 K=K+1 IF (K.EQ.1)GO TO 55 IF (K.EQ.2)GO TO 60 IF (K.EQ.3)GO TO 65 IF (K.EQ.4)GD TO 70 IF (K.EQ.5)GO TO 75 AN=AN-SIGN(1)\*0.005 55 57 WRITE(6,57) GO TO 200 DN=DN-SIGN(2)\*0.005 60 GO TO 200 65 F1=F1-SIGN(3)\*10 GO TO 200 70 P2=P2-SIGN(4)\*0.25 GO TO 200 75 AR=AR-SIGN(5)\*.005 K=0 GO TO 200 100 CONTINUE WRITE(6,57) AN=AN-SIGN(1)\*0.005 DN=DN-SIGN(2)\*0.02 P1=P1-SIGN(3)#20 P2=P2-SIGN(4)\*0.5 AR=AR-SIGN(5)\*0.02 200 CONTINUE

- 53 FORMAT(1X, "AN=", F8.6, "DN=", F8.6, "P1=", F8.3, "P2=", F8.3, "AR=", F8.6) RETURN
- END

С

С

#### SUBROUTINE OUTPUT

С

С

COMMON SP(16), PM(5), F1, F2, F3, P4, FB, FC, T1, T2, T3, TB, TC, T15, DUMMY COMMON T1R, T2R, H1, H2, H2S, H3, H4, X2, V34, CPW, CFS, TM, AN, BN, CN, DN, ANS COMMON BNS, DNS, ARS, AR, CR, U, R, CRF, DP3, DP1, DP2, DT1, DH1, CF1, WA, WP, CA COMMON HWH, STM, C11, C12, B11, B12, B13, B14, B15, X11, FAF, FAM, FAT, FAN, FAR COMMON C21, C22, B21, B22, B23, B24, X21, FBT, FB1, FBN, F2T, F2F, FBW, C31, C32 COMMON C33,C34,C35,C36,B31,B32,B33,X31,FCA1,FCA2,FCR,FCPW,FCP,C41 COMMON B41, B42, B43, X41, FDN, FD1, Y2, ZA, ZB, ZC, ZD, CF, HF, ZTOLD, K, COUNT COMMON ZTOT, CFUEL, B34, FCB

С COMPUTE AVAILABLE ENERGY OUTPUT IN THE FORM OF HOT WATER AND C THE SYSTEM SECOND LAW EFFICIENCY (ASSUMING THAT THE A. E. IN THE FUEL IS EQUAL TO THE HEATING VALUE OF THE FUEL).

- IELAVL=HWM\*CFW\*((TB-TC)-537.0\*(ALOG((TB+460)/(TC+460)))) ETTA2=(DELAVL+WA)/HF
- 50 FORMAT(1X, "SPECIFIED PARAMETERS")
- FORMAT(/, "HWM=", E15,9," TB=", FB.2," TC=", FB.2," WA=", E15,9, 75 !\* CF=\*,E15.9,///)
- FORMAT (10X, "SHADOW PRICE (",12,") =",E15.9) 100
- 200 FORMAT(10X, "MARGINAL PRICE (", I1, ")=", E15.9)
- 300 FORMAT(//, "OFTIMAL CAFITAL INVESTMENTS FOR EACH COMPONENT")

FORMAT(//10X, PURCHASE COST (DOLLARS) , 10X, AMORTIZED , 400 ! "INVESTMENT (DOLLARS/HOUR)")

- 500 FORMAT(/,5X, "TURBINE",4X,E15.9,15X,E15.9)
- FORMAT(/,5X,\*BOILER\*,5X,E15.9,15X,E15.9) 600
- FORMAT(/,5X,\*CONDENSER\*,2X,E15.9,15X,E15.9) 700
- FORMAT(/,5X, "PUMP",7X,E15.9,15X,E15.9) 800
- FORMAT(/,5X, "SYSTEM", 5X, E15.9, 15X, E15.9) 850
- ",E15.9," BTU/HOUR") 900 FORMAT(///,10X, FUEL CONSUMPTION=
- 1000 FORMAT(/,10X, FUEL COST = \*,E15.9,\* DOLLARS/HOUR\*)
- 1100 FORMAT(/,10X, TOTAL OPERATING COST= ",E15,9," DOLLARS/HOUR")
- 1150 FORMAT(/,10X, SECOND LAW EFFICIENCY=",E15.9)

1200 FORMAT(1X,///, "OFTIMAL OPERATING PARAMETERS",/)

WRITE(7,300)

C COMPUTE THE PURCHASE COST OF EACH COMPONENT AND THE SYSTEM, C ALSO COMPUTE THE AMORTIZED SYSTEM COST.

PURZA=ZA/CRF PURZB=ZB/CRF PURZC=ZC/CRF PURZD=ZD/CRF ZSYS=ZA+ZB+ZC+ZD PURSYS=ZSYS/CRF WRITE(7,400) WRITE(7,600)PURZA,ZA WRITE(7,600)PURZB,ZB WRITE(7,500)PURZB,ZB WRITE(7,500)PURZD,ZD WRITE(7,800)PURZD,ZD WRITE(7,850)PURSYS,ZSYS WRITE(7,900)HF WRITE(7,1000)CFUEL WRITE(7,1100)ZTDT

WRITE(7,1150)ETTA2 WRITE(7,1200) WRITE(7,1300) WRITE(7,1400)AN,PM(1),DN,PM(2),P1,PM(3),P2,PM(4),AR,PM(5) WRITE(7,1400)AN,PM(1),DN,PM(2),P1,PM(3),P2,PM(4),AR,PM(5) WRITE(7,1400)AN,PM(1),T2,SP(2) WRITE(7,1500)H2,SP(1),T2,SP(2) WRITE(7,1500)H2,SP(1),T2,SP(2) WRITE(7,1600)F3,SP(3),H3,SP(4) WRITE(7,1600)F3,SP(3),H3,SP(4) WRITE(7,1700)P4,SP(5),H4,SP(6) WRITE(7,1800)STM,SP(7),WP,SP(8) WRITE(7,1800)H1,SP(9),T1,SP(10) WRITE(7,2000)H2S,SP(11),BN,SP(12) WRITE(7,2100)HF,SP(13),T3,SP(14) WRITE(7,2200)TM,SP(15),CA,SP(16) RETURN END

Sample Output

### SPECIFIED PARAMETERS

HWM= .50000000E+08 TB= 275.00 TC= 150.00 WA= .125000000E+08 CF= .30000000E-05

# OPTIMAL CAPITAL INVESTMENTS FOR EACH COMPONENT

	PURCHAS	SE COST (DOLLARS)	AMORTIZED	INVESTMENT	(DOLLARS/HOUR)
80	ILER	.468234257E+0 <b>6</b>	.877976731	E+01	
TU	RBINE	.755085605E+06	.1415785518	E+02	
CO	NDENSER	.964409449E+05	.1808267728	E+01	
PU	MP	<b>.</b> 206077961E+03	.3863961768	E+00	
SY	STEM	-134038860F+07	2513228638	+02	

FUEL CONSUMPTION=	.833333333E+08	BTU/HOUR
FUEL COST =	.25000000E+03	DOLLARS/HOUR
TOTAL OPERATING COST=	.275132288E+03	DOLLARS/HOUR
SECOND LAW EFFICIENCY=	.299382012E+00	

## OPTIMAL OPERATING PARAMETERS

.

THERMODYNAMIC PARAMETER	ASSOCIATED MARGINAL PRICE
AN= .900000	.965450864E-01
DN= .890000	107344862E-04
P1= 520.000	147957416E-02
P2= 50.750	233835333E-03
AR= .823000	.102248208E-03
THERMODYNAMIC PARAMETER	ASSOCIATED SHADOW PRICE
H2= .112822187E+04	258618883E-01
T2= .281955106E+03	856497822E-01
P3= .502425000E+02	324690922E-01
H3= .250527208E+03	875040250E-02
P4= .630303030E+03	<b>.946</b> 698720E-03
H4= .253327416E+03	.129341465E+00
STM= .712092743E+05	.281779521E-02
WP= .199400773E+06	.514969035E-05
H1= .1,30856101E+04	.202751957E+00
T1= .614773211E+03	.871587850E-01
H2S= .110395864E+04	.144319003E+00
BN= .880242128E+00	.332174194E+02
HF= .833333333E+08	.30000000E-05
T3= .281320393E+03	536368936E-02
TM= .423275518E+02	232550215E-01
CA= .147657861E+04	<b>.6</b> 66627197E-03

# APPENDIX G

# OPTIMAL DESIGN DATA FOR THE COGENERATION

SYSTEM

Fue1 Cost CF $[\frac{\$}{10^6 \text{Btu}}]$	Work-Heat Ratio <u>WA</u> Q	Net Shaft Work WA [ $\frac{10^7 Btu}{Hr}$ ]	Boiler Efficiency AN	Pump Efficiency DN	Pl [psia]	P2 [psia]	Boiler Pressure Drop Coefficient AR
Required	Hot Water To	emperature, '	ГВ = 225				
2 2 2 2	0.200 0.250 0.300 0.400	0.7500 0.9375 1.1250 1.5000	0.895 0.895 0.890 0.880	0.655 0.670 0.690 0.760	350 480 680 1260	27.50 23.50 20.00 21.50	0.825 0.830 0.830 0.840
3 3 3 3	0.200 0.250 0.300 0.400	0.7500 0.9375 1.1250 1.5000	0.900 0.900 0.895 0.885	0.660 0.675 0.695 0.755	340 460 670 1250	27.00 22.75 22.00 21.50	0.820 0.825 0.830 0.845
4 4 4 4	0.200 0.250 0.300 0.400	0.7500 0.9375 1.1250 1.5000	0.905 0.900 0.900 0.890	0.655 0.675 0.690 0.760	320 480 670 1240	25.50 23.75 22.00 21.00	0.815 0.825 0.830 0.840
Required	Temperature	, TB = 250					
2 2 2 2 2 2 2 2 2	0.175 0.200 0.225 0.250 0.275 0.300 0.325	0.8750 1.0000 1.1250 1.2500 1.3750 1.5000 1.6250	0.895 0.895 0.895 0.890 0.890 0.885 0.885	0.665 0.675 0.680 0.695 0.705 0.715 0.730	340 410 500 610 740 870 1040	36.75 35.50 34.75 34.25 33.75 33.50 33.25	0.820 0.825 0.825 0.825 0.830 0.835 0.835

Table G.I. Optimized Decision variable	Table	G.1.	Optimized	Decision	Variable
--	-------	------	-----------	----------	----------

.

Fue1 Cost CF $\left[\frac{\$}{10^6 \text{Btu}}\right]$	Work-Heat Ratio <u>WA</u> Q	Net Shaft Work WA [ $\frac{10^7Btu}{Hr}$ ]	Boiler Efficiency AN	Pump Efficiency DN	P1 [psia]	P2 [psia]	Boiler Pressure Drop Coefficient AR
Required	Temperature,	TB = 250	(continued)				
2	0.350	1.750	0.880	0.755	1210	33.00	0.835
2 2	0.375 0.400	1.875 2.000	0.880 0.875	0.765	1410	33.00	0.840
3	0.175	0.875	0.900	0.665	330	36.25	0.820
3	0.200	1.000	0.900	0.680	400	35.00	0.820
3	0.225	1.125	0.900	0.680	500	34.50	0.830
3	0.250	1.250	0.895	0.700	600	34.00	0.830
3	0.275	1.375	0.895	0.710	720	33.75	0.830
3	0.300	1.500	0.890	0.720	870	33.50	0.830
3	0.325	1.625	0.890	0.735	1030	33.25	0.830
3	0.350	1.750	0.885	0.760	1200	33.00	0.835
3	0.375	1.875	0.885	0.770	1400	33.00	0.840
3	0.400	2.000	0.880	0.790	1600	33.00	0.850
4	0.175	0.875	0.905	0.670	320	35.75	0.820
4	0.200	1.000	0.905	0.675	390	34.50	0.815
4	0.225	1.125	0.900	0.680	500	34.50	0.825
4	0.250	1.250	0.900	0.705	590	33.75	0.825
4	0.275	1.375	0.900	0.705	720	33.50	0.830
4	0.300	1.500	0.895	0.725	860	33.50	0.835
4	0.325	1.625	0.895	0.730	1020	33.25	0.835
4	0.350	1.750	0.890	0.760	1200	33.00	0.835
4	0.375	1.875	0.890	0.770	1390	33.00	0.840
4	0.400	2.000	0.885	0.795	1590	33.00	0.845

Table G.1 (continued)

.

189

r

Fuel Cost CF $[\frac{\$}{10^6 \text{Btu}}]$	Work-Heat Ratio <u>WA</u> Q	Net Shaft Work WA $\left[\frac{10^7 \text{Btu}}{\text{Hr}}\right]$	Boiler Efficiency AN	Pump Efficiency DN	Pl [psia]	P2 [psia]	Boiler Pressure Drop Coefficient AR
Required	Hot Water T	emperature,	TB = 275				
2	0.20	1.1250	0.895	0.690	540	51.50	0.820
2	0.25	1.5625	0.890	0.705	790	50.25	0.835
2	0.30	1.8750	0.885	0.745	1130	50.00	0.835
3	0.20	1.1250	0.900	0.690	520	50.75	0.825
3	0.25	1.5625	0.895	0.715	780	50.25	0.835
3	0.30	1.8750	0.890	0.745	1120	50.00	0.840
4	0.20	1.1250	0.900	0.695	520	50.75	0.825
4	0.25	1.5625	0.900	0.720	780	50.00	0.830
4	0.30	1.8750	0.895	0.750	1110	50.00	0.840
Required	Hot Water T	emperature,	TB = 300				
2	0.20	1.5000	0.890	0.715	690	73.75	0.835
2	0.25	1.8750	0.885	0.735	1010	73.25	0.835
2	0.30	2.2500	0.875	0.775	1440	73.00	0.840
3	0.20	1.5000	0.895	0.720	680	73.50	0.830
3	0.25	1.8750	0.890	0.740	1010	73.00	0.835
3	0.30	2.2500	0.885	0.780	1430	73.00	0.840
4	0.20	1.5000	0.900	0.725	670	73.25	0.825
4	0.25	1.8750	0.895	0.745	1000	73.00	0.830
4	0.30	2.2500	0.885	0.785	1420	72.75	0.840

Table G.1 (continued)

$[\frac{Fuel}{Cost} \\ CF \\ [\frac{\$}{10^{6}Btu}]$	Work-Heat Ratio <u>WA</u> Q	Net Shaft Work WA [ <u>10<sup>7</sup>Btu</u> ]	Turbine Efficiency BN	$\frac{Pump}{Work}\\WP}[\frac{10^{5}Btu}{Hr}]$	Steam Mass Flow Rate STM [ $\frac{10^51bm}{Hr}$ ]	T1 [°F]	T2 [°F]
Required	Hot Water 7	Cemperature, T	B = 225				
2 2 2 2	0.20 0.25 0.30 0.40	0.7500 0.9375 1.1250 1.5000	0.852 0.872 0.888 0.919	0.840 1.141 1.587 2.669	0.4159 0.4134 0.4123 0.4116	575.5 668.8 768.8 970.6	245.4 236.7 233.1 231.8
3 3 3 3	0.20 0.25 0.30 0.40	0.7500 0.9375 1.1250 1.5000	0.856 0.876 0.891 0.923	0.814 1.090 1.552 2.650	0.4156 0.4128 0.4123 0.4120	573.4 665.6 767.8 970.0	244.4 234.9 233.1 231.8
4 4 4 4	0.20 0.25 0.30 0.40	0.7500 0.9375 1.1250 1.5000	0.860 0.874 0.891 0.922	0.775 1.139 1.564 2.626	0.4146 0.4135 0.4123 0.4116	568.8 669.0 767.8 969.0	241.2 237.2 231.1 230.5
Require	d Temperatu	re, TB = 250					
2 2 2 2 2 2 2 2	$\begin{array}{c} 0.175 \\ 0.200 \\ 0.225 \\ 0.250 \\ 0.275 \\ 0.300 \\ 0.325 \end{array}$	0.8750 1.0000 1.1250 1.2500 1.3750 1.5000 1.6250	0.848 0.865 0.876 0.884 0.891 0.903 0.908	1.063 1.277 1.568 1.892 2.267 2.627 3.092	0.5612 0.5604 0.5599 0.5595 0.5592 0.5590 0.5588	542.6 590.8 640.9 692.0 743.7 793.9 846.1	262.2 260.1 258.9 258.0 257.1 256.7 256.3

Table G.2. Selected Optimized State Variables

Fue1 Cost CF $\left[\frac{\$}{10^{6}\text{Btu}}\right]$	Work-Heat Ratio <u>WA</u> Q	Net Shaft Work WA $\left[\frac{10^7 Btu}{Hr}\right]$	Turbine Efficiency BN	Pump Work WP $[\frac{10^5 \text{Btu}}{\text{Hr}}]$	Steam Mass Flow Rate STM [ $\frac{10^51bm}{Hr}$ ]	T1 [°F]	T2 [°F]
Required	Temperature,	TB = 250	(continued)				
2 2 2	0.350 0.375 0.400	1.7500 1.8750 2.0000	0.917 0.924 0.934	3.491 4.004 4.357	0.5581 0.5587 0.5587	896.5 947.7 996.3	255.8 255.8 255.8
3 3 3 3 3 3 3 3 3 3 3 3 3 3	$\begin{array}{c} 0.175\\ 0.200\\ 0.225\\ 0.250\\ 0.275\\ 0.300\\ 0.325\\ 0.350\\ 0.375\\ 0.400 \end{array}$	0.8750 1.0000 1.1250 1.2500 1.3750 1.5000 1.6250 1.7500 1.8750 2.0000	0.854 0.869 0.874 0.888 0.897 0.903 0.910 0.918 0.926 0.934	1.030 1.243 1.558 1.834 2.188 2.625 3.059 3.439 3.949 4.357	0.5609 0.5500 0.5597 0.5594 0.5592 0.5590 0.5588 0.5587 0.5587 0.5587	540.5 589.0 640.7 690.7 741.2 793.9 845.3 895.7 946.9 996.3	261.4 259.3 258.4 257.6 257.2 256.7 256.3 255.8 255.8 255.8
4 4 4 4 4 4 4 4 4 4	$\begin{array}{c} 0.175\\ 0.200\\ 0.225\\ 0.250\\ 0.275\\ 0.300\\ 0.325\\ 0.350\\ 0.375\\ 0.400 \end{array}$	0.8750 1.0000 1.1250 1.2500 1.3750 1.5000 1.6250 1.7500 1.8750 2.0000	0.861 0.873 0.874 0.890 0.896 0.905 0.912 0.918 0.927 0.935	0.989 1.227 1.568 1.801 2.204 2.560 3.031 3.439 3.920 4.328	0.5606 0.5597 0.5597 0.5592 0.5590 0.5590 0.5588 0.5587 0.5587 0.5587	538.4 587.1 640.8 689.3 741.5 792.9 844.5 895.7 946.2 995.7	260.5 258.4 257.1 256.7 256.7 256.3 255.8 255.8 255.8

Table G.2 (continued)

.

Fuel Cost CF $[\frac{\$}{10^6 Btu}]$	Work-Heat Ratio <u>WA</u> Q	Net Shaft Work WA [ $\frac{10^7Btu}{Hr}$ ]	Turbine Efficiency BN	Pump Work WP [ <u>10<sup>5</sup>Btu</u> ]	Steam Mass Flow Rate STM [ $\frac{10^51bm}{Hr}$ ]	T1 [°F]	T2 [°F]
Required	Hot Water To	emperature, 1	TB = 275				
2	0.20	1.1250	0.872	2.090	0.7126	617.9	282.9
2	0.25	1.5625	0.895	3.014	0.7117	719.2	281.3
2	0.30	1.8750	0.912	4.148	0.7116	822.6	281.0
3	0.20	1.1250	0.880	1.994	0.7121	614.8	282.0
3	0.25	1.5625	0.898	2.932	0.7117	718.0	281.3
3	0.30	1.8750	0.914	4.084	0.7116	821.7	281.0
4	0.20	1.1250	0.880	$1.980 \\ 2.931 \\ 4.020$	0.7121	614.7	282.0
4	0.25	1.5625	0.897		0.7116	717.9	281.0
4	0.30	1.8750	0.916		0.7116	820.8	281.0
Required	l Hot Water '	Temperature,	TB = 300				
2	0.20	1.5000	0.887	3.058	0.8715	644.7	306.5
2	0.25	1.8750	0.908	4.489	0.8711	747.5	306.0
2	0.30	2.2500	0.924	6.147	0.8710	852.0	305.8
3	0.20	1.5000	0.890	3.009	0.8713	643.3	306.2
3	0.25	1.8750	0.908	4.459	0.8710	747.4	305.8
3	0.30	2.2500	0.925	6.063	0.8710	851.2	305.8
4 <sup>.</sup>	0.20	1.5000	0.894	2.960	0.8711	642.0	306.0
4	0.25	1.8750	0.910	4.410	0.8701	746.4	305.8
4	0.30	2.2500	0.926	5.980	0.8708	850.3	305.5

Table G.2 (continued)

Fuel Cost CF $[\frac{\$}{10^6}$ Btu	Work-Heat Ratio <u>WA</u> Q	Net Shaft Work WA [ <u>107Btu</u> ] Hr	Amortized Boiler Cost ZA [\$/Hr]	Amortized Turbine Cost ZB [\$/Hr]	Amortized Condenser Cost ZC [\$/Hr]	Amortized Pump Cost ZD [\$/Hr]	Total Amortized Component Cost ZTOT [\$/Hr]	Fuel Input HF [ <u>10<sup>7</sup>Btu</u> ] Hr	Second Law Efficiency <sup>N</sup> II
Require	d Hot Wat	er Tempe	erature, T	B = 225					
2 2 2 2	0.200 0.250 0.300 0.400	0.7500 0.9375 1.1250 1.5000	3.90 4.67 5.46 10.52	10.11 11.75 13.45 18.59	1.52 1.87 2.12 2.27	0.24 0.28 0.35 0.55	15.78 18.58 21.38 31.94	5.03 5.24 5.48 5.96	0.2757 0.3000 0.3216 0.3581
3 3 3 3	0.200 0.250 0.300 0.400	0.7500 0.4375 1.1250 1.5000	4.49 5.29 6.09 11.18	10.14 11.80 13.53 18.77	1.55 1.98 2.12 2.27	0.24 0.28 0.34 0.54	16.42 19.36 22.09 32.76	5.00 5.21 5.45 5.93	0.2773 0.3022 0.3233 0.3601
4 4 4 4	0.200 0.250 0.300 0.400	0.7500 0.4375 1.1250 1.5000	5.30 5.45 7.12 12.10	10.16 11.78 13.54 18.54	1.67 1.85 2.12 2.69	0.23 0.29 0.34 0.55	17.36 19.37 23.12 33.88	4.97 5.21 5.42 5.90	0.2788 0.3022 0.3251 0.3621
Requir	ed Hot Wa	ater Temp	perature,	TB = 250					
2 2 2 2 2 2 2	0.175 0.200 0.225 0.250 0.275 0.300	0.8750 1.0000 1.1250 1.2500 1.3750 1.5000	4.84 5.34 6.06 6.26 7.52 8.22	11.40 12.11 13.17 14.22 15.27 16.65	1.68 1.78 1.85 1.92 1.99 2.05	0.27 0.30 0.34 0.38 0.42 0.47	17.84 19.54 21.42 22.78 25.21 27.39	6.56 6.70 6.84 7.02 7.16 7.34	0.2741 0.2870 0.2994 0.3096 0.3210 0.3300

Table G.3. Optimized Capital Investments, Fuel Input, Second Law Efficiency

.

Fuel Cost CF [] 10 <sup>6</sup> Btu	Work-Heat Ratio <u>WA</u> Q	Net Shaft Work WA [ <u>107Btu</u> ]	Amortized Boiler Cost ZA [\$/Hr]	Amortized Turbine Cost ZB [\$/Hr]	Amortized Condenser Cost ZC [\$/Hr]	Amortized Pump Cost ZD [\$/Hr]	Total Amortized Component Cost ZTOT [\$/Hr]	Fuel Input HF [ <u>10<sup>7</sup>Btu</u> ]	Second Law Efficiency <sup>¶</sup> II
Require	d Hot Wat	er Tempe	erature, I	B = 250 (	continued	)			
2 2 2 2	0.325 0.350 0.375 0.400	1.6250 1.7500 1.8750 2.0000	10.45 12.34 16.40 20.71	17.89 19.59 21.65 25.55	2.12 2.24 2.24 2.24 2.24	0.53 0.62 0.69 0.83	30.99 34.80 40.98 49.33	7.48 7.67 7.81 8.00	0.3405 0.3486 0.3583 0.3655
3 3 3 3 3 3 3 3 3 3 3	$\begin{array}{c} 0.175\\ 0.200\\ 0.225\\ 0.250\\ 0.275\\ 0.300\\ 0.325\\ 0.350\\ 0.375\\ 0.400 \end{array}$	0.875 1.000 1.125 1.250 1.375 1.500 1.625 1.750 1.875 2.000	5.58 6.16 7.09 6.98 8.27 9.03 11.32 13.09 17.40 21.90	11.0812.1613.1414.2815.5116.6518.0419.7821.8725.55	1.72 1.83 1.88 1.95 1.99 2.05 2.12 2.24 2.24 2.24	0.27 0.30 0.34 0.38 0.42 0.47 0.54 0.62 0.70 0.83	18.65 20.44 22.45 23.60 26.19 28.21 32.02 35.74 42.21 50.52	6.53 6.67 6.80 6.98 7.12 7.30 7.44 7.63 7.77 7.95	0.2756 0.2886 0.3011 0.3113 0.3228 0.3319 0.3423 0.3506 0.3603 0.3678
4 4 4 4 4 4	0.175 0.200 0.225 0.250 0.275 0.300 0.325	0.875 1.000 1.125 1.250 1.375 1.500 1.625	6.69 7.37 7.09 8.04 9.66 10.08 12.63	11.14 12.21 13.14 14.36 15.45 16.79 18.21	1.76 1.88 1.88 1.99 2.05 2.05 2.12	0.26 0.30 0.33 0.38 0.42 0.48 0.52	19.85 21.77 22.45 24.78 27.58 29.39 33.48	6.49 6.63 6.80 6.94 7.08 7.26 7.40	$\begin{array}{c} 0.2771 \\ 0.2902 \\ 0.3011 \\ 0.3130 \\ 0.3246 \\ 0.3338 \\ 0.3444 \end{array}$

Table G.3 (continued)

195

. . .

Fuel Cost CF $[\frac{\$}{10^6}$ Btu	Work-Heat Ratio <u>WA</u> Q	Net Shaft Work WA [ <u>107Btu</u> ] Hr	Amortized Boiler Cost ZA [\$/Hr]	Amortized Turbine Cost ZB [\$/Hr]	Amortized Condenser Cost ZC [\$/Hr]	Amortized Pump Cost ZD [\$/Hr]	Total Amortized Component Cost ZTOT [\$/Hr]	Fuel Input HF [ <u>10<sup>7</sup>Btu</u> ] Hr	Second Law Efficiency <sup>¶</sup> II
Requir	ed Hot Wa	ater Temp	perature,	TB = 250	(continue	d)			
4	0.350	1.750	14.40	19.78	2.24	0.62	37.04	7.58	0.3526
4	0.375	1.875	18.86	22.12	2.24	0.70	43.93	7.72	0.3623
4	0.400	2.000	23.18	25.09	2.27	0.85	52.18	7.91	0.3697
Requir	ed Hot Wa	ater Temp	perature,	TB = 275					
2	0.20	1.1250	7.72	14.01	1.73	0.40	23.86	8.38	$0.2977 \\ 0.3198 \\ 0.3398 \\ 0$
2	0.25	1.5625	9.73	16.71	1.89	0.49	28.82	8.79	
2	0.30	1.8750	14.29	19.96	1.95	0.64	36.85	9.18	
3	0.20	1.1250	8.78	14.16	1.81	0.39	25.13	8.33	0.2994
3	0.25	1.5625	10.85	16.85	1.89	0.49	30.08	8.73	0.3216
3	0.30	1.8750	15.51	20.16	1.95	0.64	38.26	9.18	0.3398
4	0.20	1.1250	8.78	14.16	1.81	0.39	25.13	8.33	0.2994
4	0.25	1.5625	12.67	16.80	1.95	0.50	31.92	8.68	0.3234
4	0.30	1.8750	17.29	20.38	1.95	0.65	40.27	9.08	0.3437
Requir	ed Hot Wa	ater Temp	perature,	TB = 300					
2	0.20	1.5000	9.88	16.09	1.68	0.50	28.16	$10.11 \\ 10.59 \\ 11.14$	0.3062
2	0.25	1.8750	14.11	19.70	1.76	0.64	36.21		0.3277
2	0.30	2.2500	22.77	24.24	1.83	0.89	49.73		0.3452

Table G.3 (continued)

Fuel Cost CF [] 10 <sup>6</sup> Btu	Work-Heat Ratio <u>WA</u> Q	Net Shaft Work WA [ <u>107Btu</u> ] Hr	Amortized Boiler Cost ZA [\$/Hr]	Amortized Turbine Cost ZB [\$/Hr]	Amortized Condenser Cost ZC [\$/Hr]	Amortized Pump Cost ZD [\$/Hr]	Total Amortized Component Cost ZTOT [\$/Hr]	Fuel Input HF [ <u>10<sup>7</sup>Btu</u> ] Hr	Second Law Efficiency <sup>¶</sup> II
Require	ed Hot Wa	ter Temp	erature,	TB = 300	(continue	d)			
3 3 3	0.20 0.25 0.30	1.5000 1.8750 2.2500	$11.00 \\ 15.51 \\ 25.53$	16.21 19.62 24.56	$1.72 \\ 1.83 \\ 1.83$	$0.51 \\ 0.65 \\ 0.91$	29.44 37.62 52.83	$10.05 \\ 10.53 \\ 11.02$	0.3079 0.3295 0.3492
4 4 4	0.20 0.25 0.30	1.5000 1.8750 2.2500	12.68 17.28 25.17	16.37 19.86 24.75	1.76 1.83 1.95	0.51 0.66 0.94	31.32 39.63 52.81	$10.00 \\ 10.47 \\ 11.02$	0.3096 0.3314 0.3492

Table G.3 (continued)

Fue1 Cost	Work- Heat	Electricity Produced	Cost to Produce	If Market Price of Electricity is [¢/KwH]					
CF	Ratio	E	CE	3	3.5	4	4.5	5	
$\left[\frac{\$}{10^{6}\text{Btu}}\right]$	$\frac{WA}{Q}$	[10 <sup>3</sup> KwH]	[ <del>¢</del> KwH]	Net Revenue on Electricity is [\$/Hr]					
2	0.175	2.436	1.943	25.74	37.92	50.10	62.28	74.46	
2	0.225	3.131	1.965	32.42	48.08	63.73	79.39	95.02	
2	0.250	3.479 3.827	2.038	35.53	52.92	70.32	87.71 94.23	113.36	
2 2	0.300 0.325	4.175 4.523	2.079 2.187	38.45 36.77	59.33 59.39	80.20 82.00	$101.08 \\ 104.62$	121.95	
2 2	0.350	4.871 5.219	2.300 2.507	34.11 25.72	58.46 51.82	82.82 77.91	$107.17 \\ 104.01$	$131.53 \\ 130.10$	
2	0.400	5.567	2.790	11.67	39.50	67.34	94.17	123.01	
3	0.175	2.436	2.061	22.88	35.06	47.24	59.42	71.60	
3	0.225	3.131	2.150	26.60	42.26	57.91	73.57	89.22	
3	0.250	3.827	2.271	27.91	47.05	66.19	85.32	104.46	
3 3	0.300 0.325	4.175 4.523	2.331 2.455	27.92 24.64	48.80	69.67 69.87	90.55	111.42	
3 3	0.350	4.871 5.219	2.584 2.805	20.26 10.20	44.62 36.29	68.98 62.38	93.33 88.48	$117.68 \\ 114.57$	
3	0.400	5,567	3.102	-5.58	22.17	50.01	77.85	105.68	

Table G.4. Net Revenue Generated on the Sale of Electricity (TB =  $250^{\circ}$ F)

.

Fuel Cost	Work- Heat	Electricity Produced	Cost to Produce	If Marl	ket Price o	f Electri	city is	[¢/KwH]
CF	Ratio WA	E	CE	3	3.5	4	4.5	5
$\left[\frac{10^{6}}{10^{6}}\right]$	$\frac{d}{Q}$	[10 <sup>-</sup> KwH]	[ <del>KwH</del> ]	Net 1	Revenue on	Electrici	ty is [\$	5/Hr]
4	0.175	2.436	2.165	20.35	32.53	44.71	56.89	69.07
4	0.200	2.783	2.259	20.61	34.53	48.44	62.36	76.27
4	0.225	3.131	2.328	21.05	36.70	52.35	68.01	83.67
4	0.250	3.479	2.391	21.20	38.59	55.99	73.38	90.78
4	0.275	3.827	2.494	19.38	38.52	57.65	76.78	95.92
4	0.300	4.175	2.573	17.84	38.71	59.59	80.46	101.34
4	0.325	4.523	2.715	12.90	35.52	58.13	80.74	103.36
4	0.350	4.871	2.858	6.90	31.25	55.61	79.97	104.32
4	0.375	5.219	3.095	-4.96	21.14	47.23	73.33	99.42
4	0.400	5.567	3.405	-22.56	5.27	33.11	60.94	88.78

Table G:4 (continued)

.

#### REFERENCES

- Klein, S. A., Beckman, W. A., Duffie, J. A., <u>TRNSYS, A</u> <u>Transient System Simulation Program</u>, University of Wisconsin Solar Energy Laboratory Report No. 38-10, 1979.
- Eggert, R. J., Bessler, W. F., Computer Modeling Simple Thermodynamic Systems, General Electric Report No. 80CRD272, November 1980.
- Fewell, M. E., Grandjean, N. R., <u>User's Manual for</u> <u>Computer Code SOLTES-1B</u>, Sandia Publication SAND78-1315, Sandia Laboratory, Albequerque, NM, 1980.
- 4. STEAM, computer subroutine, Georgia Institute of Technology, Atlanta, GA.
- 5. Rodriguez, S. J., L. R., GASES computer code.
- Rodriguez, S. J., L. R., "Calculation of Available Energy Quantities," <u>Thermodynamics:</u> Second Law Analysis, A.C.S. Symposium Series, <u>122</u>, 1980, 39-59.
- Lewis, G. N., Randall, M., <u>Thermodynamics</u>, revised by Pitzer, K. S., Brewer, L., 2nd ed. McGraw-Hill, New York, 1961.
- 8. Pitzer, K. S., et al., <u>J. Amer. Chem. Soc.</u>, <u>77</u>, 1955, 3427.
- Wepfer, W. J., Gaggioli, R. A., "Reference Datums for Available Energy Analyses," <u>Thermodynamics: Second</u> Law Analysis, A.C.S. Symposium Series, 122, 1980, 77-92.
- Ahrendts, J., "Die Exergie Chemisch Reaktionsfahiger Systeme," VDI-Forschungesheft, 579, 1979, 39.
- 11. Sherwood, T. K., Pigford, R. L., and Wilkie, C. R., Mass Transfer, McGraw-Hill, New York, 1975.
- 12. King, C. J., Separation Processes, 2nd ed., McGraw-Hill, New York, 1980.
- 13. Callen, H. B., Thermodynamics, J. Wiley, New York, 1960.
- 14. DeGroot, S. R., <u>Thermodynamics of Irreversible Processes</u>, North Holland Publ. Co., 1951.

- 15. Denbigh, K., <u>The Principles of Chemical Equilibrium</u>, 3rd ed., Cambridge University Press, 1971.
- 16. Peters, M. S., Timmerhaus, K. D., <u>Plant Design and</u> <u>Economics for Chemical Engineers</u>, 3rd ed., McGraw-Hill, New York, 1980.
- 17. Gaggioli, R. A., et al., "Pinpointing the Real Inefficiencies in Power Plants and Energy Systems," <u>Proc.</u> Amer. Power Conf., 1975, 37,656.
- 18. Gaggioli, R. A., Petit, P. J., "Use the Second Law First," Chemtech, 1977, 7, 496-506.
- Moore, B. B., "The Feasibility and Application of Second Law Based Design Optimization Methodology to Mass Transfer Processes," M.S. Thesis, Georgia Institute of Technology, August, 1982.
- 20. Reistad, G. M., Gaggioli, R. A., "Available-Energy Costing," Thermodynamics: Second Law Analysis," <u>American Chemical Society Symposium Series</u>, 122, 1980, 143-160.
- 21. Wepfer, W. J., "Applications of Available-Energy Accounting," <u>Thermodynamics: Second Law Analysis,</u> <u>American Chemical Society Symposium Series, 122,</u> 1980, 161-186.
- 22. Evans, R. B., "Thermoeconomic Isolation and Essery Analysis," <u>Energy-The International Journal</u>, <u>5</u>, 8-9, Aug-Sept, 1980, 805-822.
- 23. Smith, M. S., "Effect of Condenser Design Upon Boiler Feedwater Essergy Costs in Power Plants," M.S. Thesis, Georgia Institute of Technology, March 1981.
- 24. Evans, et al., "Essergetic Functional Analysis for Process Design and Synthesis," Paper No. 28c, AIChE Annual Meeting, Detroit, MI, August 1982.
- 25. Wepfer, W. J., Crutcher, B. G., "Comparison of Costing Methods for Cogenerated Process Steam and Electricity," Proc. Amer. Power Conf., 43, 1070-1082, 1981.
- 26. Benedict, M., Gyflopoulos, E. P., "Economic Selection of the Components of an Air Separation Process," Thermodynamics: Second Law Analysis, American Chemical Society Symposium Series, 122, 1980, 195-203.

- 27. Wepfer, W. J., Gaggioli, R. A., "An Instructional Experiment for First and Second Law Analysis of a Gas-Fired Air Heater," <u>International Journal of Mechanical Engineering</u> <u>Education, 9, 4 (1981), 283-295.</u>
- Gaggioli, R. A., et al., "Pinpointing the Real Inefficiencies in Power Plants and Energy Systems," <u>Proc.</u> <u>Amer. Power Conf.</u>, 37 (1975), 671-679.
- 29. Gaggioli, R. A., Wepfer, W. J., "Available-Energy Accounting--A Cogeneration Case Study," Paper presented at the 85th National Meeting of the AIChE (Philadelphia, June 8, 1978).
- 30. Wepfer, W. J., Crutcher, B. G., "Comparison of Costing Methods for Cogenerated Process Steam and Electricity," <u>Proc. Amer. Power Conf.</u>, 43 (1981), 1070-1082.
- 31. El-Sayed, Y. M., Tribus, M., "The Strategic Use of Thermoeconomic Analysis for Process Improvement," Paper presented at the National Meeting of the AIChE (Detroit, August 16-19, 1981).
- 32. Clark, F. D., Lorenzoni, A. B., <u>Applied Cost Engineering</u>, Marcel Dekker, Inc., New York, 1978.
- 33. Duwell, R., Private Communication, 1981-82, Purchasing Agent, Combustion Engineering, Windsor, CT.
- 34. Hatcher, N., Private Communication, 1981-82, Energy Engineer, Combustion Engineering, Valley Forge, TN.
- 35. Humphreys, K. K., Katell, S. <u>Basic Cost Engineering</u>, Marcel Dekker, Inc., New York, 1981.
- 36. Klein, H. A., Private Communication, 1981-82, Director of Corporate Energy Management and Technical Activities, Combustion Engineering, Windsor, CT.
- 37. Peters, M. S., Timmerhaus, K. D., <u>Plant Design and</u> <u>Economics for Chemical Engineers</u>, 2nd Ed., McGraw-Hill, New York, 1968.
- 38. "Turbines and Auxiliaries," Toshiba Corp., Tokyo, Japan, 1978.
- 39. Boetler, K. "Essergy Analysis of Boilers," M.S. Thesis, Georgia Institute of Technology, Atlanta, 1982.
- 40. "STEAM," Computer Subroutine, Georgia Institute of Technology, Atlanta.
- 41. Garceau, R. M., "Thermoeconomic Optimization of a Rankine Cycle Cogeneration System," M.S. Thesis, Georgia Institute of Technology, Atlanta, 1982.
- 42. El-Sayed, Y. M., Evans, R. B., "Thermoeconomics and the Design of Heat Systems," <u>Trans. A.S.M.E., J. Engrg.</u> <u>Power</u>, <u>92</u>, 1970, 27-34.