Copyright

by

Zelong Liu

2010

# The Report Committee for Zelong Liu Certifies that this is the approved version of the following report:

# THERMOECONOMIC OPTIMIZATION OF A HEAT RECOVERY STEAM GENERATOR (HRSG) SYSTEM USING TABU SEARCH

# APPROVED BY SUPERVISING COMMITTEE:

Supervisor:		
	J. Wesley Barnes	
	I.l., D. II.,	
	John R. Howell	

# Thermo-economic Optimization of a Heat Recovery Steam Generator (HRSG) system using Tabu Search

by

Zelong Liu, B.E.; M.S.E.

## Report

Presented to the Faculty of the Graduate School of

The University of Texas at Austin

in Partial Fulfillment

of the Requirements

for the Degree of

**Master of Science in Engineering** 

The University of Texas at Austin

May 2010

## **Dedication**

To Shirong Fu, my Grandmother

## Acknowledgements

I would like to thank my supervisor, Dr. J. Wesley Barnes, for his professional guidance and generous support to my study and research at UT Austin. I shall never forget his help. I would like to thank Dr. John R. Howell for his reading and correcting to my report. I would also like to thank all the faculty and my classmates at OR/IE at UT Austin for their help and partnerships.

Especially, I would like to thank my good friends and classmates, Ms. Hongmei Huang and Dr. Yu Zhao for their unconditional help and support during this period. They are truly my life-time friends.

Finally, I would like to thank my loving wife, Sumin, for her encouragement and sacrifice to me and our family. Also, I am grateful to be blessed with my precious daughter and son, Angela and Brasen.

#### **Abstract**

## Thermoeconomic Optimization of a Heat Recovery Steam Generator (HRSG) system using Tabu Search

Zelong Liu, M.S.E

The University of Texas at Austin, 2010

Supervisor: J. Wesley Barnes

Heat Recovery Steam Generator (HRSG) systems in conjunction with a primary gas turbine and a secondary steam turbine can provide advanced modern power generation with high thermal efficiency at low cost. To achieve such low cost efficiencies, near optimal settings of parameters of the HRSG must be employed. Unfortunately, current approaches to obtaining such parameter settings are very limited. The published literature associated with the Tabu Search (TS) metaheuristic has shown conclusively that it is a powerful methodology for the solution of very challenging large practical combinatorial optimization problems. This report documents a hybrid TS-direct pattern search (TS-DPS) approach and applied to the thermoeconomic optimization of a three pressure level HRSG system. To the best of our knowledge, this algorithm is the first to be developed that is capable of successfully solving a practical HRSG system.

vi

A requirement of the TS-DPS technique was the creation of a robust simulation module to evaluate the associated extremely complex 19 variable objective function. The simulation module was specially constructed to allow the evaluation of infeasible solutions, a highly preferable capability for methods like TS-DPS. The direct pattern search context is explicitly embodied within the TS neighborhoods permitting different neighborhood structures to be tested and compared. Advanced TS is used to control the associated continuum discretization with minimal memory requirements. Our computational studies show that TS is a very effective method for solving this HRSG optimization problem.

## **Table of Contents**

List of Tables	X
List of Figures	xi
Chapter 1: Introduction	1
Chapter 2: Background	3
2.1 Heat Recovery Steam Generator (HRSG) Systems Review	3
2.1.1 Steam Turbine (ST) Simple Cycle power plant	4
2.1.2 Gas Turbine (GT) Simple Cycle power plant	5
2.1.3 Combined Cycle Gas Turbine (CCGT) power plant	6
2.1.4 Integrated Gasification Combined Cycle (IGCC) Power Plant	8
2.1.5 Heat Recovery Steam Generator (HRSG)	9
2.2 Process simulations and optimizations review	12
2.2.1 Process Simulation	12
Equation-Oriented (EO) approach	12
Sequential-Modular (SM) approach	13
2.2.2 Process Simulation/Optimization Commercial Software Packages	14
1. Company "Thermoflow" "GT PRO" and "GT MASTER"	14
2. Company GE energy "Gate Cycle"	15
3. Company GE energy "Knowledge <sup>3</sup> (Kn <sup>3</sup> TM)"	15
4. Company "Invensys" PRO/II	18
5. Company "ASPENTCH" Aspen Plus	18
6. Company "ASPENTCH" HYSYS	21
2.3 Academic research review	24
2.3.1 Tabu Search (TS) applied to continuous non-linear problems	24
2.3.2 Genetic Algorithms (GA) to the continuous non-linear problems	29
2.3.3 Direct pattern search (DPS) algorithm	36
2.3.4 Hybrid optimization algorithms	38

Chapter 3: Thermodynamics system numerical simulation	43
Chapter 4: Optimization programming	47
4.1 Thermal Economic Optimization	47
4.2 Optimizing thermal efficiency	49
4.3 Optimization Methodology	51
4.4 The Advantages of a deterministic neighborhood definition	55
4.5 The TS-DPS Pseudo-code	56
Chapter 5: Results and Discussion	59
5.1 Thermal energy efficiency	59
5.2 Thermoeconomical Ratio	61
5.3 Effect of neighborhood definition.	66
Chapter 6: Conclusions	67
References	68
Vita	72

## **List of Tables**

Table.1 "Aspen HYSYS" available solvers	
Table.2 Summary of global optimization methods (1996)	29
Table.3 Hybrid search algorithms	39
Table.4 Y.S. Teh, G.P. Rangaiah (2003) tested 20 functions	41
Table.5 Y.S. Teh, G.P. Rangaiah (2003) test results	42
Table.6 Gas turbine data at design point	44
Table.7 Variables names and meanings	45
Table.8 Variables for Best Solution Found	61
Table.9 Optimum variables for Thermo-economical ratio	64

## **List of Figures**

Figure.1 Steam Turbine (ST) simple cycle power generation	3
Figure.2 Gas Turbine (GT) simple cycle power generation	4
Figure.3 Combined Cycle Gas Turbine (CCGT) power generation	5
Figure 4 Tampa Electric IGCC Project	7
Figure.5 Tampa Electric IGCC Project	8
Figure.6 Schematic for IGCC with CO2 capture and H2 production	9
Figure.7 Heat recovery Steam generator (HRSG)	10
Figure.8 "GT PRO" simulation user interface	14
Figure.9 "PRO/II" simulation user interface	16
Figure 10 "PRO/II" optimization definition	16
Figure 11 "PRO/II" SQP optimization algorithm	17
Figure 12 "Aspen Plus" simulation user interface	19
Figure 13 "Aspen HYSYS" simulation user interface	21
Figure 14 P. SIARRY "ball" neighborhood definition	25
Figure 15 Random hyper-rectangular neighborhood definition	26
Figure 16 General flow chart of ECTS	27
Figure 17 TS application to the heat exchangers networks	28
Figure 18 Manuel Valdes HRSG with different pressure	30
Figure 19 Manuel Valdes GA convergence	31
Figure.20 Manuel Valdes GA application to three pressure HRSG	32
Figure.21 Manuel Valdes machine learning GA convergence	32
Figure 22 HYSYS simulation flow sheet of the NGL recover plant	33
Figure.23 Architecture between user, GA, MATLAB, HYSYS	33

Figure.24 Aspen plus simulator for the GQSA problem	
Figure.25 General Structure of GA for HE design	35
Figure.26 Solution strategy for the optimum of HE design	35
Figure.27 simplex move: Reflection	37
Figure.28 simplex move: Expansion	37
Figure.29 simplex move: Contraction	38
Figure.30 simplex move: Multi-contraction	38
Figure.31 GQSA is faster than pure GA optimization	40
Figure.32 Flow diagram of three pressure HRSG system	43
Figure.33 1-Δ neighborhood for 3 dimensional problems (Nb=6)	52
Figure.34 2-Δ neighborhood for 3 dimensional problems (Nb=12)	53
Figure.35 3-Δ neighborhood for 3 dimensional problems (Nb=8)	53
Figure 36 Composite of the 1- $\Delta$ and 2- $\Delta$ neighborhoods	54
Figure 37 Composite of the 1- $\Delta$ and 3- $\Delta$ neighborhoods	54
Figure 38 Pseudo code of the TS-DPS algorithm	58
Figure.39 T-Q Plot for the best thermal efficiency solution	59
Figure.40 Convergence of thermal efficiency	60
Figure.41 a Compromise between high efficiency and low cost	62
Figure.42 Two pressure configuration.	63
Figure.43 Convergence of thermoeconomic ratio	65
Figure 44 Effect of neighborhood definitions	66

### **Chapter 1: Introduction**

It is well known that a gas turbine combined with a multi-pressure level HRSG system can have thermal efficiencies in excess of 55% with comparatively low facility costs (Alessandro, et al. 2002). Single cycle gas or steam turbine systems can achieve nearly 40% thermal efficiency but only with insupportably high facility costs

Conventional thermodynamic optimization problems are very difficult to solve because the associated continuous objective function and constraints are highly nonlinear and their evaluation requires a complex simulation model. Certain combinations of system parameters can cause computational difficulties within the simulation model, stopping its execution. Care must be exercised in the coding of the simulation model to make it robust under such conditions.

Several researchers (Attala, et al. 2001; Alessandro, et al. 2002; Manuel, et al. 2003) have studied the thermoeconomic optimization of HRSG systems. Attala et al. (2001) used practical data and regression analysis to model the cost functions of the major components of a combined cycle power plant such as the HRSG, gas turbine, steam turbine, generator, and condenser. Such cost functions are invaluable in the thermoeconomic optimization of such a system. Alessandro et al (2002) applied a Nelder-Mead simplex pattern search algorithm to optimize the operations of a gas turbine combined cycle plant. Manel et al (2003) performed thermoeconomic optimization to a combined cycle gas turbine power plant using a genetic algorithm. Their work embodied the first metaheuristic approach to the area of thermoeconomic optimization. Their approach was shown to be effective on a set of selected problems with nine or fewer decision variables. The fixed cost of a *specific* gas turbine was included in their objective function.

The structure of the problem addressed in this report makes classical methods embodying nonlinear search (Bertsekas, 2003) inapplicable because no derivative information is available. In addition, the complexity of the feasible solution space makes it difficult for the search to remain feasible and once feasibility is lost it is difficult to regain. Pure direct pattern search approaches (Chelouah, et al. 2005) are also ineffective on those problems since they are easily trapped in local optima.

In this report, we propose a hybrid method combining Tabu Search (TS) and direct pattern search, TS-DPS, and apply it to the thermoeconomic optimization of a three pressure level heat recovery steam generator system. The TS-DPS local search neighborhood definition is based on a direct pattern search-coordinate descent method. TS allows the local pattern search to escape from local optima and intelligently uses memory structures to trace and control the search process.

## **Chapter 2: Background**

## 2.1 Heat Recovery Steam Generator (HRSG) Systems Review

First, this chapter introduces the concepts and applications of Gas Turbine (GT) simple cycle systems, Steam Turbine (ST) simple cycle systems, Combined Cycle Gas Turbine (CCGT) power systems, Integrated Gasification Combined Cycle (IGCC), and Heat Recovery Steam Generator (HRSG) systems. Second, this chapter presents a survey simulation and optimization investigations of such systems which includes the theoretical research and programming development in industry and academia.

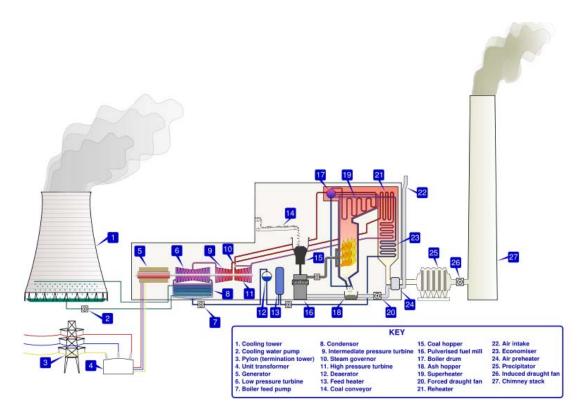


Figure.1 Steam Turbine (ST) simple cycle power generation

(Source: electricalandelectronics.org)

A power plant is an assembly of systems or subsystems to generate electricity. Major conventional power plants include a Gas Turbine (GT) simple cycle power plant, a Steam Turbine (ST) simple cycle power plant, and a Gas turbine-Steam turbine combined cycle (CCGT) power plant.

## 2.1.1 Steam Turbine (ST) Simple Cycle power plant.

A ST simple cycle power plant uses water and steam as the working medium to drive a steam turbine and to power the electricity generator. A ST simple cycle power plant is most suitable where coal is available in abundance. A ST power plant's consists primarily of: a fuel burner, a boiler (steam generator), a steam turbine (heat engine), a steam condenser, a deaerator, an electrical generator, pipes and a pumping system. An average ST simple cycle power plant's thermal efficiency is 30% - 35%.

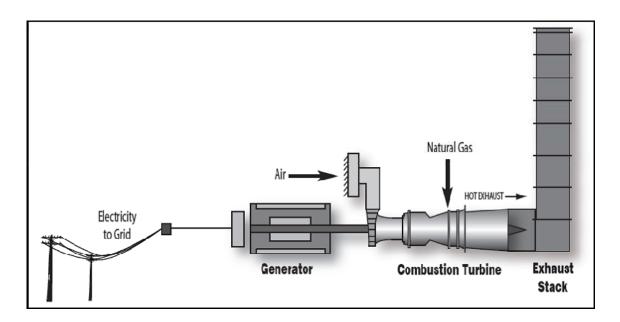


Figure. 2 Gas Turbine (GT) simple cycle power generation

(Source: www.sunriseriverenergy.com)

### 2.1.2 Gas Turbine (GT) Simple Cycle power plant

A GT obtains its power by utilizing the energy of burnt gases, from a source such as natural gas, syngas, light oil, or heavy oil, and air, which, at high temperature and pressure, expands through the turbine. A compressor is required to obtain a high pressure for the working fluid (air) which is essential for expansion. Thus, a simple gas turbine cycle consists of a compressor, a combustor, a turbine and a generator. An average GT simple cycle power plant's thermal efficiency is 35% - 43%.

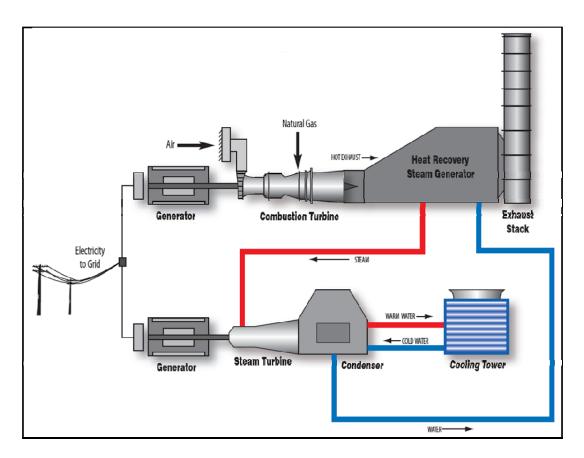


Figure.3 Combined Cycle Gas Turbine (CCGT) power generation

(Source: www.sunriseriverenergy.com)

### 2.1.3 Combined Cycle Gas Turbine (CCGT) power plant

A CCGT is a fossil fuel power plant that uses a gas turbine in conjunction with a Heat Recovery Steam Generator (HRSG). It combines the Brayton cycle (gas cycle) of the gas turbine with the Rankine cycle (steam cycle) of the HRSG. The Gas Turbine (GT) generator generates electricity and the waste heat is used to make steam to generate additional electricity via a Heat Recovery Steam Generator (HRSG) and Steam Turbine (ST). For a large scale commercial CCGT, adding a Rankine steam cycle to the Brayton gas cycle enhances the total thermal efficiency of electricity generation by 50% of the thermal efficiency of a gas turbine simple cycle. For example, a GE 9E gas turbine combined cycle thermal efficiency is 52% (heat rate - 6570 BTU/kWh) which has 53% more thermal efficiency than simple cycle which has is 34% only thermal efficiency (Heat Rate - 10100 BTU/kWh). An average CCGT power plant's thermal efficiency varies from 40% to 60% depends on plant's scale. The University of Texas at Austin has a small scale CCGT power plant. The plant equipped a Westinghouse CW251B10 gas turbine, which power output is 36180KW. The gas turbine simple cycle thermal efficiency is about 31%. The combined cycle thermal efficiency is about 40%. Right now, this plant is running as a cogeneration of heat and power plant (CHP) and the thermal efficiency (generates electricity and steam for heating) is about 73% (Ryan Reid, 2008).

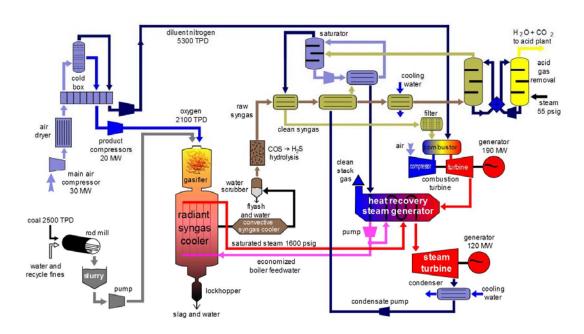


Figure.4 Tampa Electric IGCC Project

(Source: www.netl.doe.gov)

A CCGT is one of the most important fossil fuel power plants not only because the newest gas power plants in North America and Europe are of this type and usually burn natural gas (NG), light oil or heavy oil, but also because a CCGT can be used with an Integrated Gasification Combined Cycle (IGCC), burning coal. This is the most successful Clean Coal Technology (CCT). IGCC promises to be a key technology for lessening global warming problems (green house gas, carbon dioxide pollution) associated with the electrical power generation industry.

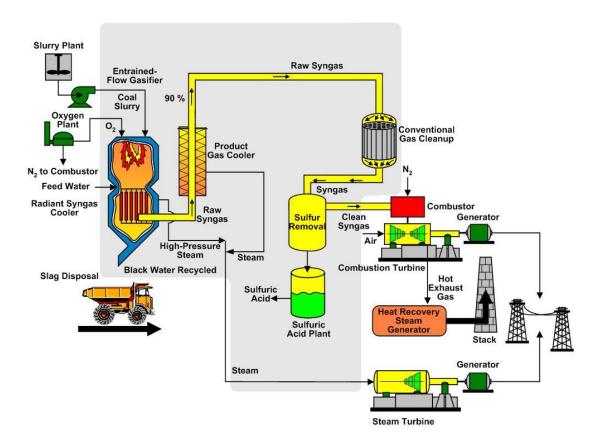


Figure. 5 Tampa Electric IGCC Project

(Source: www.netl.doe.gov)

## 2.1.4 Integrated Gasification Combined Cycle (IGCC) Power Plant

An IGCC plant provides a cleaner, economical coal-to-power option where coal or heavy fuel oil is first gasified to produce a fuel gas for a CCGT unit. Gasification is a partial oxidation process that transforms coal into a synthesis gas (syngas). The syngas stream is then cleaned and sent to a unique syngas ready gas turbine/steam turbine combined cycle system where it is used to generate electricity. An IGCC cost effectively removes pollution-causing emissions from the syngas stream before combustion. Compared with other clean coal technologies IGCC produces the lowest levels of SO<sub>x</sub>

and  $NO_x$  emissions and is the best at capturing the "Green House" gas—carbon dioxide. It can also produce hydrogen for other power needs.

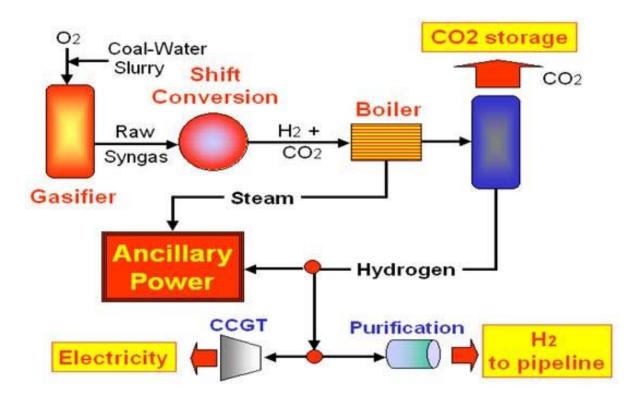


Figure.6 Schematic for IGCC with CO<sub>2</sub> capture and H<sub>2</sub> production

(Source: www.claverton-energy.com)

## **2.1.5** Heat Recovery Steam Generator (HRSG)

Advanced CCGT and IGCC power systems have a common module—a Heat Recovery Steam Generator (HRSG) system, which enables the production of over one third of the total electricity energy output. In a 10 Megawatt CCGT, the gas turbine produces about 6 Megawatts and the steam turbine produces about 4 Megawatts. An HRSG consist of three major components. They are the Evaporator, Superheater, and

Economizer. The different components are put together to meet the operating requirements of the unit.

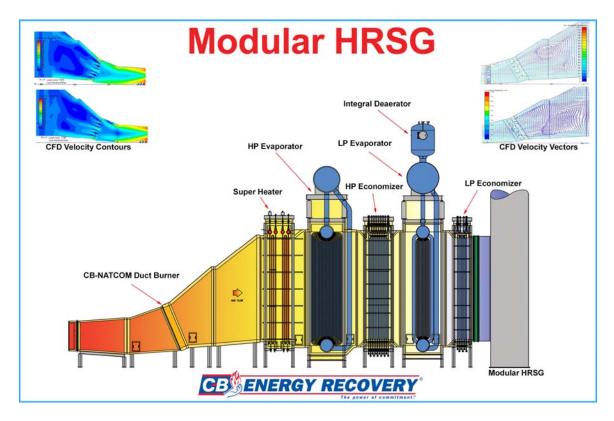


Figure.7 Heat recovery Steam generator (HRSG)

(Source: Cleaver-Brooks)

In a horizontal type HRSG, exhaust gas flows horizontally over vertical tubes. In a vertical type HRSG, exhaust gas flows vertically over horizontal tubes. A HRSG can be a single pressure and multi pressure unit. Single pressure HRSGs have only one steam drum and steam is generated at single pressure level whereas multi pressure HRSGs can employ two (double pressure) or three (triple pressure) steam drums. Triple pressure HRSG consists of three sections: an LP (low pressure) section, a reheat/IP (intermediate pressure) section, and an HP (high pressure) section. Each section has a steam drum and

an evaporator section where water is converted to steam. This steam then passes through superheaters to raise the temperature and pressure past the saturation point.

#### 2.2 Process simulations and optimizations review

Currently, the energy industry relies increasingly on the use of advanced computational modeling and simulating complex process systems. In this report, we present the computational research challenges and opportunities for the simulation and optimization of energy power generation systems from process synthesis and design to plant operations.

#### **2.2.1 Process Simulation**

Process simulation is used for the design, development, analysis, and optimization of technical processes. Process simulation software describes processes in flow diagrams where unit operations are positioned and connected by product streams. The software has to solve for mass and energy balance to find a stable operating point. The goal of a process simulation is to find optimal conditions for an examined process. This type of an optimization problem must be solved iteratively. Process simulators typically consist of unit operation models, thermodynamic calculation models, reaction models, and a physical property database. The unit operation models typically perform mass and energy balances. Engineers use process simulators to quickly predict the steady state and dynamic behavior of power plants, as well as to perform equipment costing and sizing calculations.

#### Equation-Oriented (EO) approach

The EO approach is one way to solve a steady-state process model, where all of the process equations are solved simultaneously. The greatest advantage of such an approach is their suitability for sophisticated general purpose numerical algorithms. Derivatives are calculated in an efficient and accurate manner and, in principle, the solver has full access to all variables, equations and derivative information

The EO approach offers speed and flexibility for steady-state calculations and is an excellent approach for performing dynamic simulations. It has proved to be very useful in real time optimization (on-line optimization), but often at the price of losing the robustness of the numerical methods especially developed for some unit operations. Also, to obtain the performance benefits of this optimization approach, the development, analysis and implementation are much more difficult and time consuming than with the previous ones. Moreover, for large non-convex NLP problems, no algorithms exist that solve such problems in polynomial time.

#### Sequential-Modular (SM) approach

Most steady-state simulators use the SM approach where the process flowsheet consists of unit operation models and all recycle streams. Each unit operation is solved separately. The iterative approach is needed to achieve global convergence. This sequential modular approach is essentially a "black-box" approach. The unit-specific procedures are fairly straightforward. However, because the overall flowsheet consists of black-box modules, simulation is usually performed using slow convergence techniques. Moreover, for optimization, the calculation of derivatives involves perturbing and resimulating the entire flowsheet with respect to the decision variables. This process is both time-consuming and error prone due to probable internal convergence failures involved. Another advantage with sequential based process simulators is that their graphical user interface (GUI) can make implementation of the petrochemical process models relatively less time consuming than in equation based models.

## 2.2.2 Process Simulation/Optimization Commercial Software Packages

## 1. Company "Thermoflow" "GT PRO" and "GT MASTER"

The Thermoflow Company's "GT PRO" and "GT MASTER" are two simulation packages that simulate expected performance of specific Gas Turbine and Steam Turbine Combined Cycle power plants at different operating conditions, such as different ambients and loads. Those software packages are pure SM simulations without special global optimization functions.

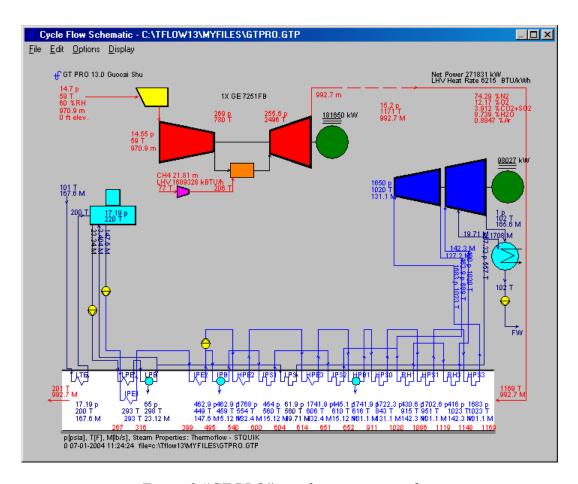


Figure.8 "GT PRO" simulation user interface

(Source: www.thermoflow.com)

#### 2. Company GE energy "Gate Cycle"

The GE energy company's "GateCycle" is design and simulation software that calculates heat balances under design and off-design conditions for any type of thermal power plant. GateCycle software predicts design and off-design performance of combined cycle plants, fossil boiler plants, nuclear power plants, cogeneration systems, combined heat-and-power plants, advanced gas turbine cycles and many other energy systems. Its component-by-component approach and advanced macro capabilities allow people to model virtually any type of system.

## 3. Company GE energy "Knowledge3 (Kn3 TM)"

The GE energy company has another optimization package called "Knowledge<sup>3</sup> (Kn<sup>3</sup> TM)", which provides accurate modeling technology, unique optimization and state-of-the-art control. The optimization engine provides sophisticated, multi-objective optimization, allowing several different goals to be addressed simultaneously. The optimization iteratively updates inputs, progressively driving the calculation efficiently and accurately towards the best set. The optimization technology is based on a genetic algorithm (GA). GAs are known to be able to find excellent solutions to complex optimization problems but can be time and effort intensive.

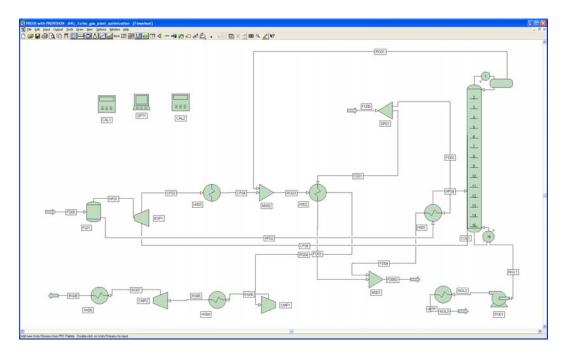


Figure.9 "PRO/II" simulation user interface

(Source: iom.invensys.com)

## Flowsheet Optimization

#### General Information

The optimization algorithm within PRO/II is a powerful tool which allows the operating conditions of a single unit or an entire process flowsheet to be optimized. Typical applications are the minimization of heat duty or the maximization of profit. Most generally, the optimization problem can be formulated as:

(1)

$$\begin{array}{lll} \text{minimize} & f\left(x_1,x_2,...,x_n\right) & \text{objective function} \\ \text{such that} & h_i\left(x_1,x_2,...,x_n\right)=0 \ \ i=1,...,m_1 & \text{specifications} \\ & g_i\left(x_1,x_2,...,x_n\right)\leq 0 \ \ i=1,...,m_2 & \text{constraints} \\ & x_{i,mini}\leq x_i\leq x_{i,maxi} \quad i=1,...,m_1 & \text{bounds} \end{array}$$

where n is the number of variables, m1 is the number of specifications and m2 is the number of constraints.

Figure.10 "PRO/II" optimization definition

(Source: iom.invensys.com)

Define  $x_k = (x_{1,k}, x_{2,k}, ..., x_{n,k})$  as the vector of the optimization variables which define the state of the system.

- Set the cycle counter k:=1 and solve the flowsheet at x1.
- 2. Perturb each optimizer variable by some amount hi and resolve the flowsheet. Use the base case flowsheet solution and the n additional flowsheet solutions to approximate the first derivatives of the objective function, specifications and constraints via finite differences.
- If k≥ 2 use the first order derivatives at the previous and current cycles to approximate the second order derivatives.
- Solve the flowsheet at xk+1 = xk + αdk.
- 6. If the flowsheet solution at  $X_{k+1}$  is not a sufficient improvement as compared to the flowsheet solution at  $X_k$  reduce the search step  $\alpha$  and return to step 4.
- Let xk+1 be the new base case. Set k:=k+1 and return to step 2.

Various tests are included after the solution of the quadratic approximation (step 3) and after each "non derivative" flowsheet solution (step 4) to determine whether the convergence tolerances are satisfied.

The quadratic programming algorithm used in step 3 automatically determines which of the constraints are binding or active i.e. which of the inequality constraints  $g_i(x) \leq 0$  are satisfied as equality constraints  $g_{i,A}(x) = 0$  at the current value of the optimizer variables. In addition, the quadratic programming algorithm ensures that the optimizer variables do not exceed their bounds and determines which variables are exactly at a bound (e.g.,  $x_1 = x_1, \max_i x_i = x_1$ ).

#### Termination Criteria

- 1. Is the relative change in the objective function at consecutive cycles less than 0.005 (or the user defined value RTOL for the objective function)?
- 2. Is the relative change in each variable at consecutive cycles less than 0.0001 (or the user defined values RTOL for each variable)?
- 3. Has the maximum number of cycles been reached?
- 4. Does the scaled accuracy of the solution fall below 10-7 (or the user defined value SVERROR)? The scaled  $KT\Sigma = \nabla f^T d + \sum_i \left| \lambda_i h_i \right| + \sum_i \left| \mu_i g_i \right|$  accuracy, which is also known as the Kuhn-Tucker error, is calculated from:
- 5. Is the relative error for each specification less than 0.001 (or the user defined value)?
- 6. Is the relative error for each constraint less than 0.001 (or the user defined value)?

Figure.11 "PRO/II" SQP optimization algorithm

(Source: iom.invensys.com)

#### 4. Company "Invensys" PRO/II

The Invensys Operations Management Company's simulation and optimization package, **PRO/II**, performs all mass and energy balance calculations needed to model most steady-state processes within the chemical, petroleum, natural gas, solids processing and polymer industries. PRO/II runs in an interactive Windows®-based GUI environment. PRO/II solves process flowsheets using an SM approach. This technique solves each individual process unit, applying the best solution algorithms available. Additionally, PRO/II applies several advanced techniques known as Simultaneous Modular Techniques, to enhance simulation efficiency.

**PRO/II** uses **Successive Quadratic Programming (SQP)** to solve the nonlinear optimization problem. SQP is similar to the direct linear approximation method where the successive quadratic method approximates the general function to a quadratic function. In each iteration of the successive quadratic programming method, a new quadratic programming problem is solved using the solution obtained from the previous iteration.

#### 5. Company "ASPENTCH" Aspen Plus

The AspenTech company's process simulation and optimization software, "Aspen Plus", is the most popular process flowsheet simulator (Advanced System for Process Engineering) was developed by MIT's Energy Laboratory at 1970s. Aspen Plus is a **Steady-State** commercial simulator, which also provides both the SM and EO simulation solution approaches.

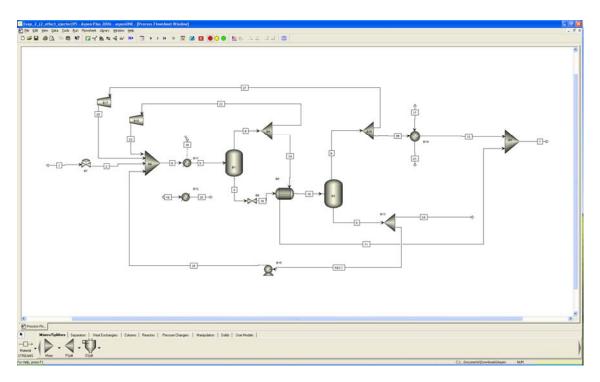


Figure.12 "Aspen Plus" simulation user interface

(Source: www.aspentech.com)

This sophisticated software package can be used in almost every aspect of process engineering from design stage to cost and profitability analysis. It has a built-in model library for many options including distillation columns, separators, heat exchangers, and reactors. User models are created with Fortran subroutines or Excel worksheets which are added to its model library. Using Visual Basic to add input forms for user models makes them indistinguishable from the native built-in ones. Aspen Plus has a built-in property databank for thermodynamic and physical parameters.

Aspen Plus Optimization Algorithm. Two optimization algorithms are available in Aspen Plus, the COMPLEX method and the SQP (successive quadratic programming) method. The COMPLEX method uses the well-known Complex algorithm, a feasible path "black-box" pattern search. The method can manage inequality constraints and bounds on decision variables. Equality constraints must be specified as

design specifications. The COMPLEX method frequently takes many iterations to converge, but does not require numerical derivatives. It has been widely used for all kinds of optimization applications for many years and offers a well-established and reliable option for optimization convergence.

The SQP method is a state-of-the-art, quasi-Newton nonlinear programming algorithm. It can converge tear streams [Aspen Plus User Guide, 2000], equality constraints, and inequality constraints simultaneously with the optimization problem. A tear stream is a recycle stream with component flows, total mole flow, pressure, and enthalpy all determined by iteration. The SQP method usually converges in only a few iterations, but requires numerical derivatives for all decision and the tear stream variables. The trade-off is the number of derivative evaluations versus the time required per derivative evaluation.

Other than the standard SQP solver, Aspen Plus uses several variants of the SQP algorithms solver which are DMO, LSSQP (Large-scale Sparse Successive Quadratic Programming algorithm), SRQP, and OPTRND for NLP (Nonlinear Programming). It performs the optimization by solving a sequence of quadratic programming subproblems. DMO offers various options for controlling the line search and trust region methods to improve efficiency and robustness, particularly for large problems. DMO is also useful for solving cases with no degrees of freedom, such as equation-oriented simulation and parameter estimation. LSSQP implements a variant of a class of successive quadratic programming (SQP) algorithms, for large-scale optimization. It performs the optimization by solving a sequence of quadratic programming subproblems.

Other than Steady-State simulators (PRO/II and Aspen Plus), dynamic simulation tools provide a continuous view of a process in action by calculating the transient behavior of the plant over time. Typical applications include plant startup, upset,

shutdown and transient analysis and the evaluation of control schemes. Well-known commercial dynamic simulators include Aspen HYSYS Dynamics® (Aspen Technology Inc.) and the EO-based packages, Aspen Dynamics® (Aspen Technology Inc.)

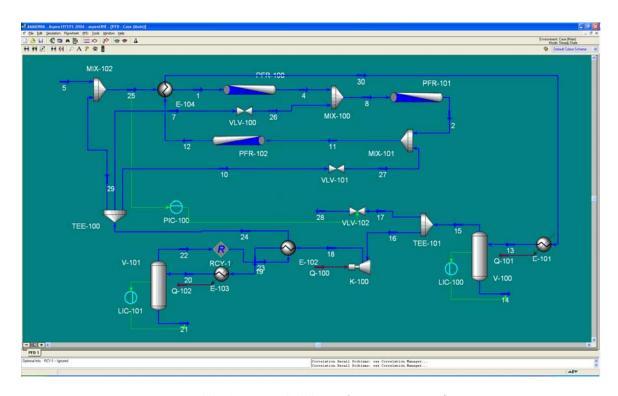


Figure.13 "Aspen HYSYS" simulation user interface

(Source: www.aspentech.com)

#### 6. Company "ASPENTCH" HYSYS

The Aspentch **HYSYS** package contains a multi-variable steady state Optimizer. The BOX, Mixed, and Sequential Quadratic Programming (SQP) methods are available for constrained minimization with inequality constraints. The original and the Hyprotech SQP methods can manage equality constraints. The Fletcher-Reeves and Quasi-Newton methods are available for unconstrained optimization problems.

The **Box method** is a sequential search technique that solves problems with non-linear objective functions, subject to non-linear inequality constraints. No derivatives are required. It manages inequality constraints but not equality constraints. This method is inefficient in terms of the required number of function evaluations. It generally requires a large number of iterations to converge to the solution. However, if applicable, this method is very robust.

The **Mixed method** attempts to take advantage of the global convergence characteristics of the BOX method and the efficiency of the SQP method. It starts the minimization with the BOX method using a very loose convergence tolerance (50 times the desired tolerance). After convergence, the SQP method is then used to locate the final solution using the desired tolerance.

The Sequential Quadratic Programming (SQP) Method manages inequality and equality constraints. SQP is considered by many to be the most efficient method for minimization with general linear and non-linear constraints, provided a reasonable initial point is used and the number of primary variables is small. It minimizes a quadratic approximation of the Lagrangian function subject to linear approximations of the constraints. The second derivative matrix of the Lagrangian function is estimated automatically. A line search procedure utilizing the "watchdog" technique [Aspen Plus online manual, 2006] is used to force convergence.

The **Quasi-Newton method of Broyden-Fletcher-Goldfarb-Shanno (BFGS)** method is similar to the Fletcher-Reeves method. It calculates the new search directions from approximations of the inverse of the Hessian Matrix.

The **Fletcher-Reeves conjugate gradient** method is efficient for general unconstrined minimization.

The discretization algorithm can be either a **stochastic method** or a **Branch and Bound Method**.

Solver	Type of Optimization	Method
FEASOPT	Steady state or dynamic	Reduced space
Nelder-Mead	Steady state or dynamic	Reduced space
HYPSQP	Steady state or dynamic	Reduced space
SRQP	Steady state	Full space
Open NLP – reduced space	Steady state or dynamic	Reduced space
Open NLP – full space	Steady state	Full space

Table.1 "Aspen HYSYS" available solvers

#### 2.3 Academic research review

### 2.3.1 Tabu Search (TS) applied to continuous non-linear problems

TS is an advanced metaheuristic optimization method that uses memory structures to escape from local optima and to prevent cycling (Glover, et al. 1993). TS starts from an initial incumbent solution and examines a neighborhood of adjacent solutions reachable in one iteration of the search. The best nontabu neighboring solution is selected as the new incumbent, and the next iteration begins. A solution attribute captures some characteristic of the solution that can be used to prohibit the search from returning to previously visited tabu solutions for a specified number of moves, the tabu tenure.

In recent times, TS has experienced many significant improvements in its algorithmic techniques as exemplified in references (Battiti, et al. 1994; Carlton et al. 1996; Harwig, et al. 2001) and has been shown to be very effective in the solution of complex combinatorial optimization problems (Colletti, et al. 1999; Barnes et al. 2004).

Tabu Search (TS) was originally used primarily to solve discrete combinatorial optimization problems, such as the traveling salesman problem (TSP). In recent years, more applications of TS to continuous optimization problems have been published.

N. Hu (1992) was the first researcher to adapt TS to continuous optimization. He proposed a tabu search with a random move neighborhood definition to global optimization problems with continuous variables.

P. Siarry, and G. Berthiau (1997) proposed a continuous variable optimization tabu search algorithm with the "ball" neighborhood definition of N. Hu (1992), and successfully applied TS to the Goldstein-Price 2 variable problem [L. C. W. Dixon and G. P. Szego, 1978] and the Hartmann 3 variables problem [K. Schittkowski and W. Hock, 1987].

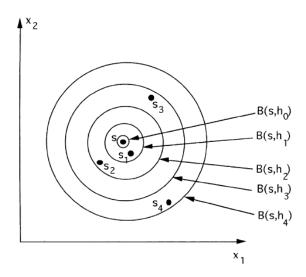


Figure.14 P. SIARRY "ball" neighborhood definition

Franze and Speciale (2001) proposed the DOPE algorithm, which was based on pattern search and tabu search, and applied it to the minimization of multidimensional functions with multiple local minima and with variables defined over continuous finite ranges. Further, the function's analytical form is unknown (hence gradient and Hessian matrix are not available) and its evaluation has a high computational cost. Their algorithm uses a Variable move step, a limited 2N directions neighborhood definition where N is the number of variables, and a monotonic reduction of the step size when no favorable point is found in the neighborhood).

Chelouah and Siarry (2000) proposed an Enhanced Continuous Tabu Search (ECTS) for the global optimization of multiminima functions which emphasized diversification and intensification strategies (Glover, 1993; Battiti et al., 1994). They used a random hyper-rectangular neighborhood to simplify the neighborhood evaluation.

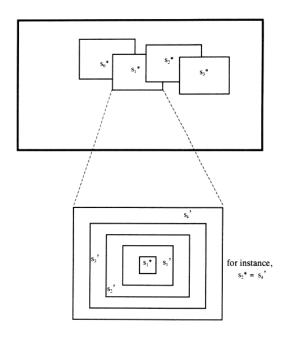


Figure.15 Random hyper-rectangular neighborhood definition

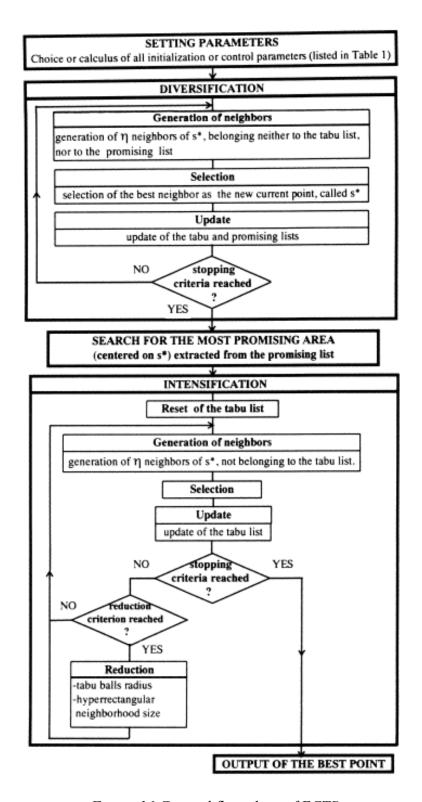


Figure.16 General flow chart of ECTS

Y. S. Teh and Rangaiah (2003), applied an enhanced continuous Tabu Search (ECTS) to the phase equilibrium calculations via Gibbs free energy minimization. They compared ECTS with a Genetic Algorithm (GA) to the same benchmark set of problems. The results show that while both TS and GA locating the global minimum, TS converges faster than GA thus reducing the computational time and number of function evaluations.

Lin and Miller (2004) implemented TS for heat exchanger network (HEN) synthesis and compare their approach to others presented in the literature using a random subset strategy to generate neighboring solutions. Figure 17 shows the solution (10 exchangers with heat duty(kW)) to a HEN problem with 5 hot streams, 5 cold streams, 1 hot utility and 1 cold utility. The objective is to minimize the annualized cost expressed as the sum of the utility costs, fixed charges for each heat exchanger and an area-based cost for each heat exchanger. The area of a heat exchanger is a highly nonlinear function of the temperature difference and heat load. In their case studies, the global optimal solution was found more than 90% of the time, demonstrating the potential of TS to solve other optimization problems in chemical engineering.

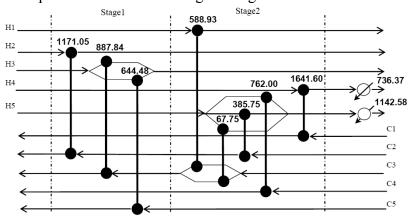


Figure. 17 TS application to the heat exchangers networks

### 2.3.2 Genetic Algorithms (GA) to the continuous non-linear problems

As presented in Table 2, Elwakeil and Arora (1996) summarized the attributes of the most popular global optimization methods at that time.

Table I. Characteristics of global optimization methods<sup>2</sup>

	Class	Can Solve		Attempts to	Phases		Uses	Gradients	
Method		Cont.	Disc.	0/1	find all x*	Local	Global	LS?	Needed?
Evtushenko	D	_/			Yes		/	a	b
Zooming	D	./	_/		No	•/	•	Yes	b
Golf	D	<b>y</b> /	•		No	3/		Yes	Yes
Tunnelling	D	<b>v</b> /			No	./	٠/٠	Yes	b
Pure R.S.	S	<b>y</b> /	·/	./	No	v	\$/	No	No
Multistart	S	<b>Y</b> /	3/	3/	Yes	_/	3/	No	No
Clustering	S	<b>.</b> //	./	3/	Yes	./	./	Yes	b
CRS	S	./	./	3/	No	./	./	d	No
SA	S	./	./		No	v	./	No	No
Accept. Rej.	Š	.\/	./	./	No		./	No	No
Stoch. Integ.	Š	./	./	.\'	No		./	No	No
Genetic	Š	v	.//	./	No		./	No	No
Tabu Search	e	e	$\checkmark$	$\checkmark$	No	$\checkmark$	$\checkmark$	f	f

D deterministic methods

local minimization procedure can be used to find the best feasible move

Table.2 Summary of global optimization methods (1996)

Focusing on Combined Cycle Gas Turbine (CCGT) power generation systems, Valdes, Duran, and Rovira (2003) performed a thorough investigation of the use of Genetic algorithms for global thermoeconomic optimization.

S stochastic methods

a use of a local minimization is not essential

b depends on the local minimization procedure used

c the 'Tunnelling Phase' is considered as a global phase

d CRS uses a special local minimization method

e the method is essentially deterministic. Random elements are used for continuous problems

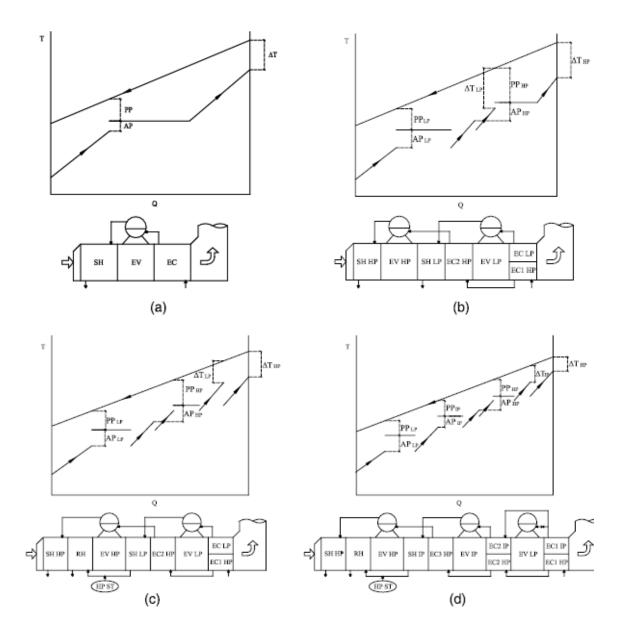


Figure.18 Manuel Valdes HRSG with different pressure

An illustrated in Figure 18, a tuned genetic algorithm was applied to a single pressure CCGT power plant and to two and three pressure levels in the heat recovery steam generator (HRSG). The variables considered for the optimization were the thermodynamic parameters that establish the configuration of the HRSG. Two different

objective functions were proposed: one minimizes the cost of production per unit of output and the other maximizes the annual cash flow. The results obtained with both functions are compared in order to find the better optimization strategy. Figure 19 shows the GA evolution of the maximum cash flow value corresponding to each generation (the maximum is the 100% reference value). Figure 20 illustrates the system studied and Figure 21 shows the convergence rate of the GA used.

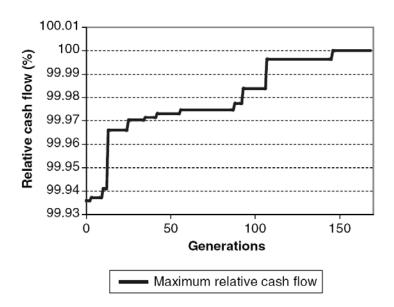


Figure.19 Manuel Valdes GA convergence

Rovira, Valdés and Casanova (2005) used a GA to solve the non-linear equations applied to Combined Cycle Gas Turbine simulation. Their methodology combined genetic-based machine learning (GBML) and GA, using a population of possible solution processes.

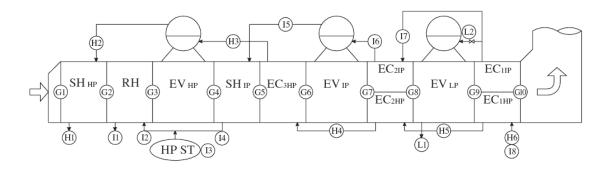


Figure.20 Manuel Valdes GA application to three pressure HRSG

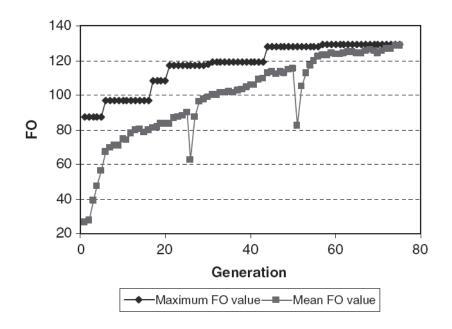


Figure.21 Manuel Valdes machine learning GA convergence

Mehrpooya, Gharagheizi, Vatani (2006) used Aspen HYSYS and GA to optimize a natural gas liquids (NGL) recovery unit pictured in Figures 22 and 23.

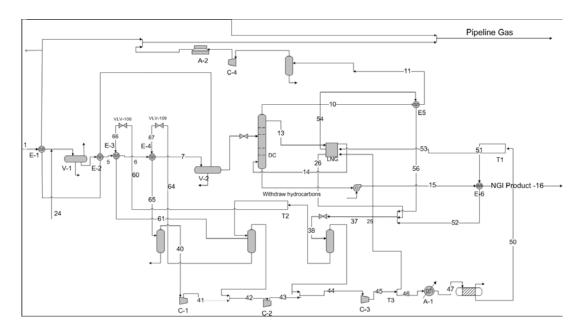


Figure.22 HYSYS simulation flow sheet of the NGL recover plant

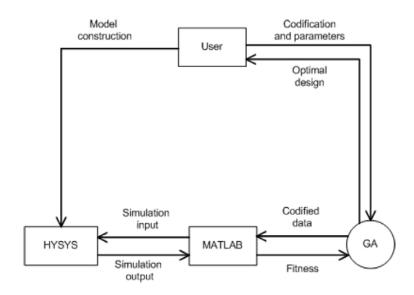


Figure.23 Architecture between user, GA, MATLAB, HYSYS

Jang, Hahn, and Hall (2005) used a Genetic/quadratic search algorithm (GQSA) for plant economic optimizations using a process simulator. By coupling a regular GA with an algorithm based upon a quadratic search, the required number of objective

function evaluations for obtaining an acceptable solution decreased significantly in most cases. Figure 24 illustrates the system that was studied.

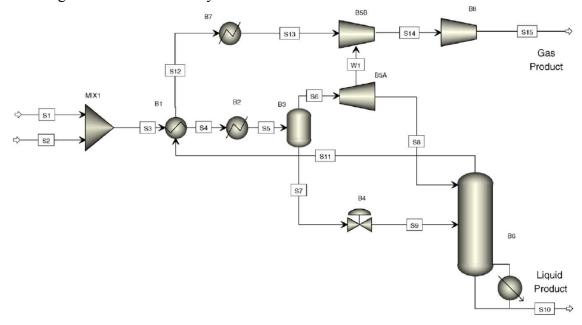


Figure.24 Aspen plus simulator for the GQSA problem

Mohagheghi and Shayegan (2009) used a GA to perform the thermodynamic optimization of design variables and heat exchangers layout in a HRSG for CCGT. A new method was introduced for modeling the steam cycle in advanced combined cycles by organizing the non-linear equations and their simultaneous solutions using hybrid Newton methods.

Ponce-Ortega, Serna-González and Jiménez-Gutiérrez (2009) presented an approach based on GAs for the optimal design of shell-and-tube heat exchangers. The examples analyzed, as illustrated in Figures 25 and 26, show that GAs provide a valuable tool for the optimal design of heat exchangers.

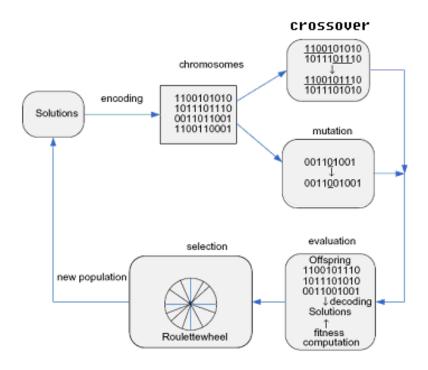


Figure.25 General Structure of GA for HE design

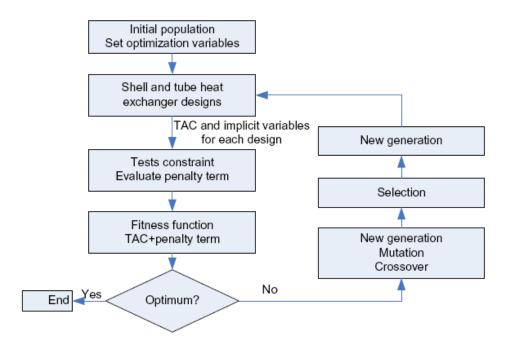


Figure.26 Solution strategy for the optimum of HE design

#### 2.3.3 Direct pattern search (DPS) algorithm

Direct pattern search, as defined in this report, requires only objective function evaluations. Direct pattern search methods like the coordinate descent method (Fermi, et al. 1996), evolutionary operation (Box, 1957), the Hook and Jeeves technique (Hooke, et al. 1961) and the very popular Nelder-Mead simplex method (Nelder, et al. 1965; Margaret, et al. 1995) date from the early 1960s. These methods were largely ignored until 1990 when McKinnon described a convergent form of the Nelder-Mead algorithm for strictly convex functions in two dimensions (Mckinnon, et al. 1998). Since that time little additional work has been focused on the Nelder-Mead approach.

Since 1990, newly developed computer hardware and software techniques brought about an increase in the use of direct pattern search methods (Wright, 1995). In 2003, Tamara et al. (2003) proved that the coordinate descent search method possesses strong convergence properties. Unlike classical combinatorial optimization problems (Carlton, et al. 1996), the solution space topology of many engineering problems is relatively smooth in its contours. These convergence properties and a smooth solution space, along with the very simple implementation of the coordinate descent method led us, in the research documented in this report, to select it to be our basic method of neighborhood generation for the associated TS methodology.

**Nelder-Mead simplex method**. The most famous simplex-based direct search method was proposed by Nelder and Mead in their 1965 paper. The Nelder-Mead method is based on the idea of creating a sequence of changing simplices which are deliberately modified so that the simplex "adapts itself to the local landscape".

The Nelder–Mead simplex algorithm is a very powerful local deterministic algorithm, making no use of the objective function derivatives. A "simplex" is a geometrical figure consisting, in n-dimensions, of (n + 1) points. If any point of a simplex

is taken as the origin, the n other points define vector directions that span the n-dimension vector space. As illustrated in Figures 27, 28, 29 and 30, through a sequence of elementary geometric transformations (reflection, contraction and extension), the initial simplex moves, expands or contracts.

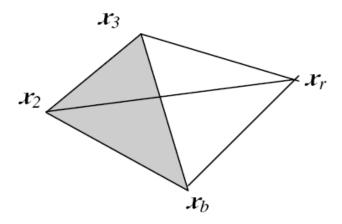


Figure.27 simplex move: Reflection

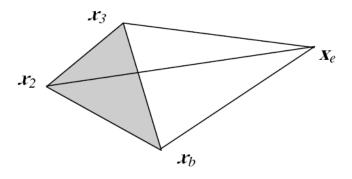


Figure.28 simplex move: Expansion

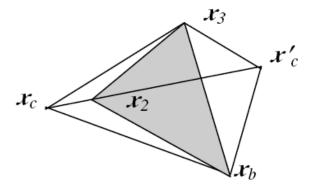


Figure.29 simplex move: Contraction

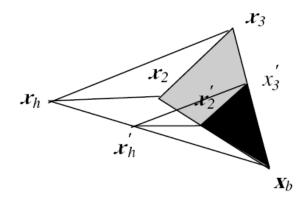


Figure.30 simplex move: Multi-contraction

# 2.3.4 Hybrid optimization algorithms

Commercial process simulators, such as ASPEN Plus, PRO/II, or HYSIS, have experienced rapid development and found widespread application in the power generation process industries. The main reason is that these process simulators can provide process engineers with rigorous descriptive thermodynamic models. When using a process simulator for process optimization, convergence of the process flowsheet is

required to evaluate the value of the objective function. Since the process flowsheet consists of multiple independent units, convergence is achieved by separate unit convergence and by applying feed back techniques for converging streams. This characteristic of process simulators can cause difficulties for gradient-based optimization because information required for computing the gradient may not be readily available and the nonlinear characteristics in the system may cause multiple local optima to be present. Gradient-free optimization techniques (Black-Box solvers) such as GA, TS, and Simulated Annealing (SA) are commonly applied to problems with such properties.

When applying those black-box solvers to optimization problems involving a process simulator, the evaluation complexity requires as few as possible objective function evaluations.

Hybrid approaches which are combined with two complementary algorithms (in terms of global exploration and local exploitation), generally have better performance than pure Black-Box algorithms.

The most common hybrid approaches are shown the Table.3:

	Global Search			
Local Search	TS	GA	SA	
Simplex search (Nelder-Mead)	TS/NM	GA/NM	SA/NM	
Pattern search				
Gradient descent				
Conjugate gradient method				
Newton method	TS/NR	GA/NR		
Quasi-Newton method (QN)	TS/QN	GA/QN		
Finite Difference Estimates				

Table.3 Hybrid search algorithms

Chelouah and Siarry (2003) proposed a **Continuous Hybrid Algorithm (CHA)**, which is a **GA/Nelder-Mead hybrid algorithm** for the global optimization of

multiminima functions. Their main contribution was the introduction of two concepts: diversification and intensification. In a diversification phase, they start with a large population and a high mutation probability to homogeneously cover the whole search space and detect a promising subspace. The intensification phase is then performed inside this promising subspace by using a local search.

Chelouah and Siarry (2003) also proposed a **Continuous Tabu Simplex Search** (CTSS) ,i.e., a **Tabu Search/Nelder-Mead hybrid algorithm**. They concluded that generally hybrid methods achieve better solutions than "pure" methods, and converge more quickly. Among pure global methods, the GA was the least accurate, and the TS was the fastest.

Jang, Hahn and Hall (2005) proposed a genetic/quadratic hybrid search algorithm (GQSA) for optimizing plant economics when a process simulator models the plant. As shown in Figure 31, the GQSA quadratic search reduces the required number of objective function evaluations for convergence to an optimum.

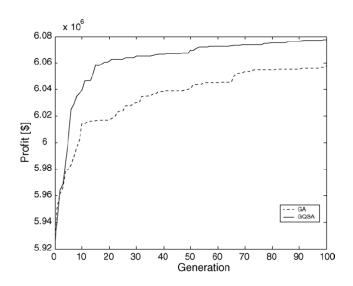


Figure.31 GQSA is faster than pure GA optimization

Number	Mixture	Feed	Pressure and temperature	Model	Reference
(a) Selec	ted examples for VLE				
1	Methane (1), propane (2)	$F = 1.0 \text{ mol}, z_I = \{0.68, 0.32\}$	100 bar, 277.6 K	SR K	Hua et al. (1998)
2	Carbon dioxide (1), methane (2)	$F = 1.0 \text{ mol}, z_i = \{0.20, 0.80\}$	60.8 bar, 220K	PR	Hua et al. (1998)
3	Hydrogen sulfide (1), methane (2)	$F = 1.0 \text{ mol}, z_i = \{0.0187, 0.9813\}$	40.53 bar, 190 K	SR K.	Hua et al. (1998)
4	Nitrogen (1), methane (2), ethane (3)	$F = 1.0 \text{ mol}, z_i = \{0.15, 0.30, 0.55\}$	76 bar, 270 K	PR	Hua et al. (1998)
5	Methane (1), carbon dioxide (2), hydrogen sulfide (3)	$F=1.0\ mol,\ z_i=\{0.4989,0.0988,0.4023\}$	48.6 bar, 227.55 K	PR	Sun and Seider (1995)
6a	Benzene (1), acetonitrile (2), water (3)	$F=1.0036\ mol,\ z_i=\{0.34359,\ 0.30923,\ 0.34718\}$	0.1 atm, 300 K	Ideal (V) NRTL (L)	Castillo and Grossmann (1981)
6b	Benzene (1), acetonitrile (2), water (3)	$F = 1.0036 \ mol, \ z_i = \{0.34359, \ 0.30923, \ 0.34718\}$	0.1 atm, 300 K	Ideal (V) UNI- FAC (L)	-
7	Nitrogen (1), argon (2), oxygen (3)	$F = 9.38529 \text{ mol}, z_i = \{0.78112, 0.00930, 0.20958\}$	607.95 kPa, 100.79 K	PR	PRO/II (1993)
8	Methane (1), ethane (2), propane (3), $i$ -butane (4), $n$ -butane (5), $i$ -pentane (6), $n$ -pentane (7), $n$ -hexane (8), $n$ -pentadecane (9)	$F = 0.96890 \text{ mol}, z_i = \{0.61400, 0.10259, 0.04985,$	19.84 atm, 314 K	SR K	Castillo and Grossmann (1981)
9	Mixture of ten hydrocarbons (see Teh and Rangaiah, 2002 for details)	F = 35.108 mol	3998.95 kPa, 287.48 K	PR	Hyprotech (1998)
10	Mixture of 11 chemicals (see Teh and Rangaiah, 2002 for details)	F = 10.0  mol	101.325kPa, 303.15 K	Ideal (V) NRTL (L)	Hyprotech (1998)
(b) Selec	ted examples for LLE				
11a	n-Butyl-acetate (1), water (2)	$F=1.0\ mol,\ z_i=\{0.50,0.50\}$	1.0 atm, 298 K	NRTL	Heidemann and Mandhane (1973)
11b	n-Butyl-acetate (1), water (2)	$F = 1.0 \text{ mol}, z_i = \{0.50, 0.50\}$	1.0 atm. 298 K	UNIFAC	McDonald and Floudas (1997)
12	Toluene (1), water (2)	$F = 1.0 \text{ mol}, z_i = \{0.50, 0.50\}$	1.0 atm, 298 K	NRTL	Castillo and Grossmann (1981)
13	Furfural (1), 2,2,4-trimethyl pentane (2), cyclohexane (3)	$F = 1.0 \text{ mol}, \ z_i = \{0.10, \ 0.10, \ 0.80\}$	1.0 atm, 298 K	UNIQUAC	Prausnitz, Anderson, Grens, Eckert, Hsieh & O'Connell, (1980)
14	Benzene (1), acetonitrile (2), water (3)	$F = 1.0036 \text{ mols}, z_i = \{0.34359, 0.30923, 0.34718\}$	1.0 atm, 333 K	NRTL	Castillo and Grossmann (1981)
15	Toluene (1), water (2), aniline (3)	$F = 0.9987 \; mol, \; z_i = \{0.29989, \; 0.20006, \; 0.50005\}$	1.0 atm, 298 K	NRTL	Castillo and Grossmann (1981)
(c) Selec 16	ted examples for VLLE Benzene (1), acetonitrile (2), water (3)	$F=1.0036\ mol,\ z_i=\{0.34359,\ 0.30923,\ 0.34718\}$	0.769 atm, 333 K	Ideal (V) NRTL (L)	Castillo and Grossmann (1981)
17	Methanol (1), methyl acetate (2), water (3)	$F=1.0\ mol,\ z_i=\{0.15,0.45,0.40\}$	0.965 atm, 325 K		McDonald and Floudas (1997)
18	Ethanol (1), benzene (2), water (3)	$F=1.0 \ mol, \ z_i = \{0.20, \ 0.35, \ 0.45\}$	1.0 atm, 338 K	Ideal (V) UNI- FAC (L)	Prokopakis and Seider (1983)
19	$Ethylene\ glycol\ (1),\ dodecanol\ (2),\ nitromethane\ (3),\ water\ (4)$	$F=1.0 \ mol, \ z_i=\{0.30, 0.10, 0.50, 0.10\}$	0.43 atm, 350 K	Ideal (V) UNI- FAC (L)	McDonald and Floudas (1997)
20	2,2,4-Trimethyl pentane (1), furfural (2), cyclohexane (3), benzene (4)	$F=1.0 \text{ mol}, \ z_i = \{0.10,  0.30,  0.40,  0.20\}$	10.0 kPa, 288 K	Virial (V), UN- IQUAC (L)	Wu and Bishnoi (1986)

Table.4 Y.S. Teh, G.P. Rangaiah (2003) tested 20 functions

As summarized in Table 4 and 5, Teh and Rangaiah (2003) tested TS/Nelder-Mead (TS/NM), TS/ Quasi-Newton method (TS/QN), GA/Nelder-Mead (GA/NM), and GAQuasi-Newton method (GA/QN) hybrid algorithms on 20 global continuous optimization functions.

Number	Number of function evaluations (computation time is seconds)				
	TS-QN	TS-NM	GA-QN	GA-NM	
1	1412 (0.13)	2710 (0.25)	20017 (1.39)	20 677 (1.52)	
2	1349 (0.14)	1498 (0.15)	20018 (1.59)	20 204 (1.62)	
3	1187 (0.13)	1349 (0.17)	20024 (1.51) <sup>a</sup>	20 176 (1.56) <sup>a</sup>	
4	1777 (0.21)	3407 (0.38)	20238 (2.09)	21 308 (2.24)	
5	1511 (0.18)	5499 (0.56)	20027 (2.06)	23 213 (2.43)	
6a	1616 (0.14)	2155 (0.17)	20089 (1.14)	21 064 (1.38)	
6b	1648 (0.17)	1782 (0.14)	20088 (1.41)	20 189 (1.57)	
7	1894 (0.29)	2474 (0.34)	20054 (2.68)	20 609 (2.71)	
8	10 040 (3.84)	11 765 (3.74)	20515 (4.85)	22 856 (5.99)	
9	Trivial	Trivial	Trivial	Trivial	
10	12 631 (3.46)	18 632 (3.77)	21 579 (3.95)	22 455 (4.01)	
11a	1425 (0.09)	1528 (0.07)	20018 (1.04)	20 160 (1.05)	
11b	1369 (0.13)	1441 (0.11)	20024 (1.36)	20 138 (1.44)	
12	1367 (0.07)	1468 (0.11)	20026 (1.02)	20 154 (1.05)	
13	1571 (0.13)	1451 (0.33) <sup>b</sup>	20028 (1.50) <sup>c</sup>	20 885 (1.69)°	
14	1557 (0.12)	2771 (0.19)	20033 (1.30)	20 917 (1.50)	
15	1719 (0.12)	1877 (0.12)	20 069 (1.20)	20 241 (1.77)	

Example number and details	Computation time (s)			
	TS-QN <sup>a</sup>	GA-QN <sup>a</sup>	Literature	
1 (VLE, SRK)	0.13	1.39	0.643 <sup>b</sup>	
2 (VLE, PR)	0.14	1.59	0.484 <sup>b</sup>	
3 (VLE, SRK)	0.13	1.51	0.290 <sup>b</sup>	
4 (VLE, PR)	0.21	2.09	4.977 <sup>b</sup>	
11a (LLE, NRTL)	0.09	1.04	0.23°	
11b (LLE, UNIFAC)	0.13	1.36	0.37°	
17 (VLLE, UNIFAC)	0.95	2.17	8.8°	
19 (VLLE, UNIFAC)	2.43	3.33	1493.3°	

Table.5 Y.S. Teh, G.P. Rangaiah (2003) test results

The test results indicate that the performance of TS/QN and GA/QN is better than that of TS/M and GA/NM, respectively. Additionally, this study showed that TS/QN required less objective function evaluations than GA/QN for mathematical functions and Gibbs free energy minimization.

# **Chapter 3: Thermodynamics system numerical simulation**

The three pressure level HRSG system of Figure.32 schematically pictures the configuration that was used to test the TS-DPS algorithm developed in the research documented in this report. There are two major reasons for this selection: (1) this system is widely used in the gas turbine power generation industry (Alessandro, et al. 2002) and a successful optimization method for this system will contribute to the solution of similar practical problems, and (2) it is typical of the type of complex problems with highly nonlinear objective and constraint functions that are encountered in the power generation industry.

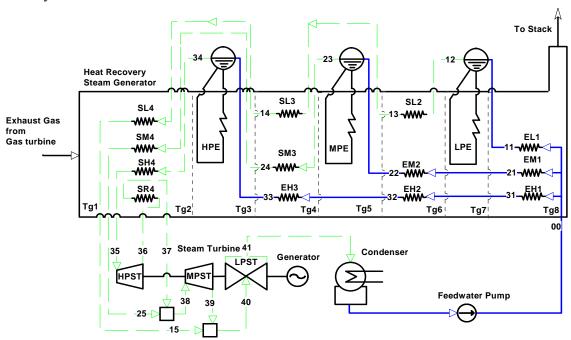


Figure.32 Flow diagram of three pressure HRSG system

Figure.32 pictures the flow of water and steam within a sophisticated three pressure HRSG system which includes 16 heat exchangers, 2 stream mixers, 3

evaporators (HPE, MPE, LPE), 3 steam turbines (HPST, MPST, LPST), 1 generator, 1 condenser and 1 feed water pump. Heat exchangers EL1, EM1, EM2, EH1, EH2, EH3 are economizers for the three water streams (—), respectively. Heat exchangers SL2, SL3, SL4, SM3, SM4, SH4 are the super heaters for the three steam streams (—), respectively. Heat exchanger SR4 is re-heater of the steam exhaust from the high pressure steam turbine.

The fixed parameters for the gas turbine are given in Table 6.

Parameter	Input data
Ambient temperature (°C)	25
Ambient pressure (bar)	1.01325
Compressor isentropic efficiency	0.85
Compressor ratio	20
Turbine isentropic efficiency	0.91
Combustor chamber efficiency	0.95
Combustor chamber pressure loss (%)	4
Turbine inlet temperature (°C)	1430
Inlet air mass (kg/s)	300
GT work outputW <sub>gt</sub> (MW)	105.3
GT thermal efficiencyET <sub>gc</sub>	0.382
fuel massG <sub>f</sub> (kg/s)	5.69
GT exhausted gas temperatureT <sub>g</sub> (°C)	503.15

Table.6 Gas turbine data at design point

Before HRSG system optimization, a simulation code for the HRSG system must be constructed that will evaluate both the system thermal efficiency and the ratio of cash flow over a fixed investment. The construction of such an evaluation code has been well described (Manuel, et al. 2004). Table 7 lists the 19 independent decision variables that constitute the input data for the HRSG simulator:

$\mathbf{x}_1$	PLP	pressure of low pressure evaporator
x <sub>2</sub>	PMP	pressure of middle pressure evaporator
X3	PHP	pressure of high pressure evaporator
X4	DTAL	sub cool temperature of low pressure water
X5	DTAM	sub cool temperature of middle pressure water
x <sub>6</sub>	DTAH	sub cool temperature of high pressure water
X7	DTPL	pinch temperature of low pressure stream
X8	DTPM	pinch temperature of middle pressure stream
X9	DTPH	pinch temperature of high pressure stream
X <sub>10</sub>	DTEM1	approach temperature at outlet of EM1
x <sub>11</sub>	DTEH1	approach temperature at outlet of EH1
X <sub>12</sub>	DTEH2	approach temperature at outlet of EH2
X <sub>13</sub>	DTSL2	approach temperature at outlet of SL2
X <sub>14</sub>	DTSL3	approach temperature at outlet of SL3
X <sub>15</sub>	DTSL4	approach temperature at outlet of SL4
x <sub>16</sub>	DTSM3	approach temperature at outlet of SM3
X <sub>17</sub>	DTSM4	approach temperature at outlet of SM4
X <sub>18</sub>	DTSH4	approach temperature at outlet of SH4
X19	DTSR4	approach temperature at outlet of SR4

Table.7 Variables names and meanings

The HRSG code must properly manage a large number of restrictions which are partitioned into soft and hard constraints. Many of the components, like air, water, steam, and gas, of the HRSG system are limited to a specific operational range. These hard

constraints can not be violated. Other soft constraints are enforced through the use of penalty functions.

## **Chapter 4: Optimization programming**

#### 4.1 Thermal Economic Optimization

In the thermal economics arenas, the thermal energy efficiency, the cost of production per unit of output and the annual cash flow are most widely used measures of effectiveness in simulation and optimization problems (Manuel, et al. 2003). In this report, the quantity and temperature of the gas turbine exhaust hot gas are fixed and the primary focus is on designing a system which will maximize the thermal energy efficiency.

The goal is to achieve greater steam turbine electricity generation while requiring a lower investment of fixed facilities associated with the HRSG. To achieve this goal, we define another objective function, detailed in Equation (1), to be a ratio of profit divided by cost, the thermoeconomic ratio. The numerator of Equation (1) captures the profit derived from the level of generated electricity in Watts ( $W_{st}$ ) by the steam gas turbine over K years where there are H hours of operation per year and the profit per Watt-hour is P. The denominator of Equation (1) is the total cost of the HRSG system,  $C_{tot}$ , composed of the sum of four component costs: (i) the cost of the steam turbine,  $C_{st}$ , (ii) the cost of the condenser,  $C_{con}$ , (iii) the cost of the generator,  $C_{gen}$ , and (iv) the cost of the rest of the components that make up the HRSG system,  $C_{hrsg}$ .

Maximize 
$$f(x) = \frac{W_{st} * K * H * P}{C_{tot}}$$
 (1)

where the components of  $C_{tot}$  are defined as follows (Attala, et al. 2001):

$$C_{hrsg} = 1700 \left[ \sum_{l} \left( \frac{Q_{econ}}{\Delta T_{econ}} \right)^{0.6} + \sum_{l} \left( \frac{Q_{evap}}{\Delta T_{evap}} \right)^{0.6} + \sum_{l} \left( \frac{Q_{sh}}{\Delta T_{sh}} \right)^{0.6} + \sum_{l} \left( \frac{Q_{lte}}{\Delta T_{lte}} \right)^{0.79} \right]$$
(2)

$$C_{st} = 319728A^{0.261} + 823.7W_{st}^{1.543} (3)$$

$$C_{cond} = 162S^{1.01} \tag{4}$$

$$C_{gen} = 3082W_{st}^{0.58} \tag{5}$$

 $Q_{econ}$ ,  $Q_{evap}$ ,  $Q_{sh}$ , and  $Q_{lte}$  is the heat energy in Watts and  $\Delta T_{econ}$ ,  $\Delta T_{evap}$ ,  $\Delta T_{sh}$ , and  $\Delta T_{lte}$  are the temperature differences at the economizers, the evaporators, the superheaters, and the feed water pre-heaters, respectively. In addition, A is the area of the steam turbine final section in square meters and S is the area of the heat exchanger surface of the condenser in square meters. The decision variables,  $x_i$ , i = 1,..., 19, determine the values of  $Q_{econ}$ ,  $Q_{evap}$ ,  $Q_{sh}$ ,  $Q_{lte}$ ,  $\Delta T_{econ}$ ,  $\Delta T_{evap}$ ,  $\Delta T_{sh}$ ,  $\Delta T_{lte}$ , A, S, and  $W_{st}$  by means of the complex relationships presented in detail in Equations (2) through (5). These complex relationships can not be analytically solved. This forces the use of a deterministic emulation, an implementation of those relationships to achieve a solution.

Historically, only thermal efficiency optimization has been performed on systems like that given in Figure 32. Such limited activities ignore the significant benefits that may be achieved by a thermoeconomics optimization. Nevertheless, a thermal efficiency optimization provides a starting point for the more comprehensive thermoeconomic optimization. In the next section we describe how such an optimization is performed.

#### 4.2 Optimizing thermal efficiency

The definition of thermal efficiency is;

Maximize 
$$f(x) = \frac{W_{gt} + W_{st}}{G_f * LHV}$$
 (6)

where  $W_{gt}$  is the electricity generated (Watts) by the gas turbine;  $G_f$  is the input mass flow of fuel to the gas turbine (in kilograms per second). LHV is the low heating value (in joules per kilogram) of the fuel (Rydstrand, et al. 2004).

Equations 7 through 15 stipulate physical relationships (constraints) that must be satisfied in the optimization of Equation 6:

$$20 \ge x_1 \ge 3.0, 60 \ge x_2 \ge 20, 200 \ge x_3 \ge 60 \text{ (bars)}, i = 1, ..., 3$$
 (7)

$$x_i \ge 3.0$$
 (degrees Celsius),  $i = 4, ..., 9$  (8a)

$$300 \ge x_i \ge 10$$
 (degrees Celsius),  $i = 10, ..., 19$  (8b)

$$T_{15} \ge T_{14} \ge T_{13} \ge T_{12} > T_{11} \ge T_{00}$$
 (9)

$$T_{25} \ge T_{24} \ge T_{23} > T_{22} \ge T_{21} \ge T_{00} \tag{10}$$

$$T_{35} \ge T_{34} > T_{33} \ge T_{32} \ge T_{31} \ge T_{00}$$
 (11)

$$T_{g1} > T_{g2} > T_{g3} > T_{g4} > T_{g5} > T_{g6} > T_{g7} > T_{g8}$$
 (12)

$$T_{37} \ge T_{36}$$
 (13)

$$D_{r36}, D_{r39}, D_{r41} \ge 90\%$$
 (14)

$$T_{g8} \ge T_{dw} \tag{15}$$

where the  $T_{ij}$  are the flow temperatures (in Kelvin degrees) at the designated specific locations pictured in Figure 32. In like manner, the  $T_{gi}$  are the exhaust gas temperatures

(in Kelvin) at their designated locations in Figure 32. Finally, Dr is the dryness of the steam at steam turbine outlet points of 36, 39 and 41 and  $T_{\rm dw}$  is the dew point temperature in degrees Kelvin.

Once again, the decision variables,  $x_i$ , i=1,...,19, determine the values of the intermediate variables, i.e., the temperatures (the  $T_{ij}$ ,  $T_{gi}$ ,  $T_{dw}$ ), the steam quality ( $D_{r36}$ ,  $D_{r39}$ ,  $D_{r41}$ ) and  $W_{st}$ , in accordance with the mathematical equations presented in detail above (Attala, et al., 2001).

## 4.3 Optimization Methodology

The values of the 19 decision variables associated with Equations 6 through 15 are obtained in the following way:

The definition of the neighborhood of an incumbent solution is essential to the TS optimization of a problem with continuous decision variables. Hu (1992) and Siarry et al. (1997) employed a "neighboring hypersphere" of radius r about an incumbent solution, s, where all s' satisfying the relation,  $\|$  s'-s  $\|$   $\leq$  r, are neighbors of s. The next iteration's incumbent solution is obtained by randomly generating k neighbors and selecting the best of them. Chelouah (2005) employed a similar neighborhood construct by formulating concentric hypercubes around the incumbent solution with a similar random neighbor selection method. Neither of these methods use the available approximate objective function derivative information and do not allow an efficient tabu memory structure, i.e., using random step sizes to discretize the continuous solution space is not conducive to an efficient tabu memory structure.

Rather than depending on randomization, our neighborhood definition borrows from basic concepts associated with coordinate direct pattern search. Many neighborhood definitions are possible in this context. One such neighborhood is the m- $\Delta$  neighborhood that was used in this research. Figures 33 through 37 illustrate the m- $\Delta$  neighborhood for a three parameter problem for m = 1, 2, 3 where m is the number of parameters that are simultaneously perturbed. In general, the cardinality of a m- $\Delta$  neighborhood is N<sub>b</sub>=  $\binom{n}{m} 2^m$ 

In Figure.33 each iteration consists of a single variable being incremented or decremented by a fixed amount,  $\Delta$ .

As illustrated in Figure.34, larger composite neighborhoods are easily defined by the superimposition of 2 or more unique m- $\Delta$  neighborhoods

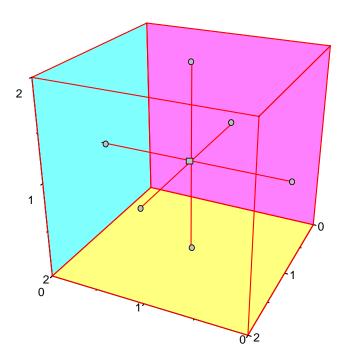


Figure.33 1- $\Delta$  neighborhood for 3 dimensional problems ( $N_b$ =6)

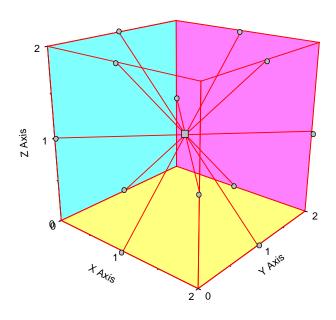


Figure.34 2- $\Delta$  neighborhood for 3 dimensional problems ( $N_b$ =12)

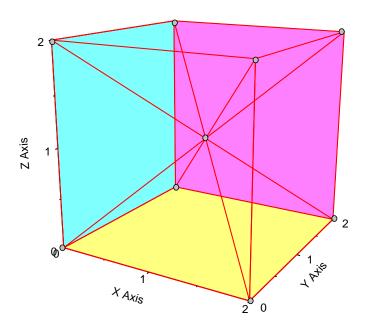


Figure.35 3- $\Delta$  neighborhood for 3 dimensional problems (N<sub>b</sub>=8)

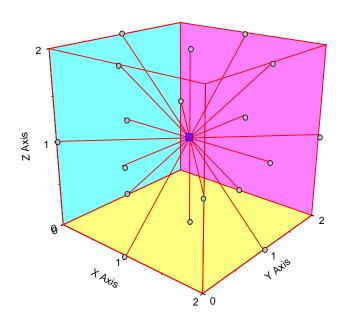


Figure.36 Composite of the 1- $\Delta$  and 2- $\Delta$  neighborhoods ( $N_b$ =6+12=18)

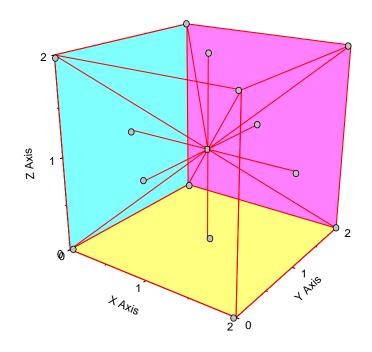


Figure.37 Composite of the 1- $\Delta$  and 3- $\Delta$  neighborhoods ( $N_b$ =6+8=14)

### 4.4 The Advantages of a deterministic neighborhood definition

In classical TS methodology, the neighborhood definition is often the most important factor in yielding excellent solutions quickly (Barnes, et al. 2003). In applying TS to continuous optimization problems, this can be even more important because the neighborhood selection is complicated by the additional requirement to specify the step size,  $\Delta$ , dynamically during the search process. Siarry, et al. (1997) studied the relationship between  $\Delta$  and the speed of convergence for a GA applied to a continuous optimization problem. Smaller step sizes yielded more precise answers but at the cost of more computational effort.

A dynamic  $\Delta$  also makes the implementation of an effective and efficient TS memory structure more challenging, i.e., preventing repetitions of a previously visited solution within a specified number of iterations is a more complex undertaking in a continuous solution space. To make these problems tractible, the following stipulations are imposed:

- $\Delta$  is limited to 3 specific values, i.e.,  $\Delta$ =5, 1, or 0.1.
- A modified form of adaptive TS [Harwig, J., Barnes, J.W., More, J., 2001]
   is employed where the tabu tenure is decreased (increased) after a specified number of consecutive improvements (disimprovements) occur.

#### 4.5 The TS-DPS Pseudo-code

In this section, a description of the TS-DPS algorithm is given using both verbal descriptions and the psuedo-code presented in Figure 38. In early computational studies, the best solution from the thermal efficiency TS-DPS optimization was used as the initial incumbent solution for the thermoeconomic ratio optimization. However, this proved ineffective because that solution to the thermal economics problem was dramatically dissimilar from good solutions to the thermal efficiency problem. After some additional empirical experimentation, it was found that an acceptable starting solution for the thermoeconomic problem was

Initial empirical experimentation led to the conclusion that the composite 1- $\Delta$  and 2- $\Delta$  neighborhood yielded a robust effective search. The initial tabu tenure was set to 3000 iterations, the initial discretization factor,  $\Delta$ , was set to 5.0 and the solution representation used in the tabu memory structure was a vector of the 19 parameter values,  $x_i$ ,  $i=1,\ldots,19$ , joined with a simple hashing value,  $\Pi_{i=1}^{19}i*x_i$ . At the start of the algorithm, the incumbent solution  $X_i$ , the initial step size  $\Delta$ , the step coefficient k, the interaction counter IT, the neighborhood implementation time, and the tolerance Eps are initialized. After initialization, the TS-DPS algorithm performs iterations until the maximum time allowed is exceeded or the tabu memory is fully filled. We use as simple a neighborhood definition (1- $\Delta$ ) as possible as long as the global best solution,  $X^*$ , is updated before time,  $T_1$ d (obtained from empirical experimentation). After  $T_1$ d time units have passed, the 1- $\Delta$  and 2- $\Delta$  neighborhood definition are implemented.

In each iteration, all neighboring solutions are considered and the best nontabu solution becomes the new incumbent solution. If all neighboring solutions are tabu, the neighborhood definition is incrementally expanded (while maintaining the same cardinality) until the best solution in the new neighborhood is not tabu, whereupon that best solution becomes the new incumbent solution. The neighborhood definition is returned to the default structure, and the iterations continue. If after 100 such expansions, the algorithm fails to find a non tabu best solution, execution terminates.

Each new best nontabu solution is compared with the global best solution and we retain the number of nonimprovements in Cnt\_nonimprovements. When Cnt\_nonimprovements = 10, the new neighborhood definition is incrementally expanded again using a different step coefficient and step size. After 100 such expansions, the neighborhood definition is returned to the default structure (k=1,  $\Delta=1.0$ ).

Each incumbent solution is placed in the tabu memory structure and, if the current solution is the best found so far, it is recorded. The algorithm terminates when the time limit is exceeded or the tabu memory is fully filled.

```
Set all required physical parameter values (Table 1)
Set initial incumbent solution, X_I = X_0; Set best solution found so far, X^* = X_I
Set step size, \Delta=5.0; Set Iteration Counter, IT = 0;
                                                              Set step size coefficient, k = 1
Set 1-\Delta neighborhood implementation time to T 1d=50.0 second
While (maximum time not exceeded) and (tabu memory is not fully filled)
   IT = IT + 1
    If (Current time < T_1d) Then
         Implement One-∆ neighborhood definition
     Else
         Implement One-Δ and Two-Δ neighborhood definition
     End If
     Evaluate all solutions in neighborhood of X_{\rm I}, X_{\rm i} \in N_{\rm I}
     If (one or more X_i are not tabu)
       Select the best non-tabu X_j, X_{j,Best}
     End If
     // Dynamic Neighborhood Management
     If (all X_i are tabu) Then
              While (k \le 100)
                   k=k+1, define new neighborhood, i.e., X_j \in N_I, with \Delta = 0.1*k
                   Evaluate all neighborhood solutions in new neighborhood
                   Select the best neighbor X_{j,Best} which is not tabu
              End while
              If (k = 101) Then Stop
     Else
         If (Cnt_nonimprovements > 10) Then reset Cnt_nonimprovements=0
              While (k \le 100)
                   k=k+1, define new neighborhood, i.e., X_i \in N_{I_i} with \Delta = 0.1*k
                   Evaluate all neighborhood solutions in new neighborhood
                   Select the best neighbor X_{j,Best} which is not tabu
              End while
              If (k = 101) Then set k = 1; \Delta = 1.0
         End If
     End If
     Set X_{\rm I} = X_{\rm j,Best},
     Place X_{\rm I} into the tabu memory structure
     If X_{\rm I} is best solution found so far, X^* = X_{\rm I}
     If X^* has not improved, reset nonimprovement counter Cnt_nonimprovements +1
} End While
```

Figure. 38 Pseudo code of the TS-DPS algorithm

# **Chapter 5: Results and Discussion**

# 5.1 Thermal energy efficiency

The TS-DPS algorithm was applied to the problem of Figure 39 with thermal efficiency as objective function. The best thermal efficiency achieved was 55.2% which is consistent with the results of previous research (Alessandro, et al. 2002). Figure 39 gives the T-Q plot for that configuration where the temperature of HRSG exhausted gas is approximately 100°C. The thermal efficiency of this system is much higher than the efficiency of typical current gas turbine combined cycle power generation systems with the same turbine inlet temperature to the gas turbine. This is partially due to the fact that practical systems are rarely designed solely for thermal efficiency. In most cases, a multicriteria objective function drives the system design.

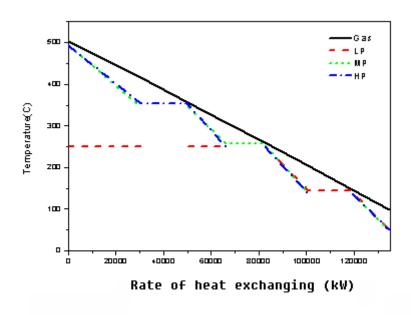


Figure.39 T-Q Plot for the best thermal efficiency solution

Figure.40 presents a plot of how quickly improved thermal efficiencies were achieved during the algorithm's search. The best solution found is given in Table 8. All pinch temperatures, sub-cool temperatures and most approach temperatures are at their lower bounds (denoted with a \* in the table).

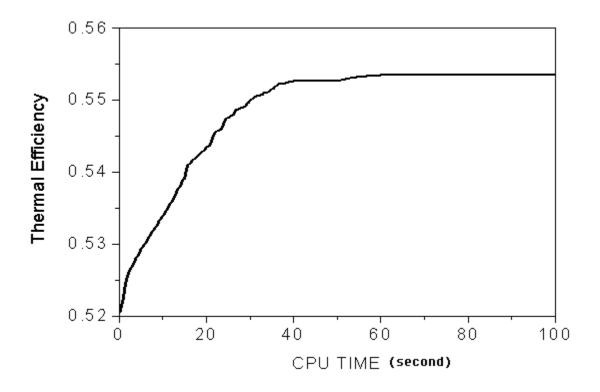


Figure.40 Convergence of thermal efficiency

## 5.2 Thermoeconomical Ratio

The solution stated in Section 4.6 is used as the initial solution for the TS-DPS algorithm when applied to the problem of optimizing the thermoeconomic ratio. The initial solution's thermoeconomic ratio was 0.76855, less then 50% of the best found thermoeconomic ratio of 1.822, reflecting the fact that high thermal efficiency is always associated with very high facility expenditures in an HRSG.

	Name	Meaning of variables	Lower	Upper	Optimum
			Bound	Bound	
$\mathbf{x}_1$	PLP	pressure of low pressure evaporator (bar)	3	20	4.1
<b>x</b> <sub>2</sub>	PMP	pressure of middle pressure evaporator (bar)	20	60	44.7
X <sub>3</sub>	PHP	pressure of high pressure evaporator (bar)	60	200	173.8
X <sub>4</sub>	DTAL	sub cool temperature of low pressure water (°C)	3	-	3*
X <sub>5</sub>	DTAM	sub cool temperature of middle pressure water (°C)	3	-	3*
x <sub>6</sub>	DTAH	sub cool temperature of high pressure water (°C)	3	-	3*
X <sub>7</sub>	DTPL	pinch temperature of low pressure stream (°C)	3	-	3*
<b>X</b> <sub>8</sub>	DTPM	pinch temperature of middle pressure stream (°C)	3	-	3*
X9	DTPH	pinch temperature of high pressure stream (°C)	3	-	3*
X <sub>10</sub>	DTEM1	approach temperature at outlet of EM1 (°C)	10	300	10*
x <sub>11</sub>	DTEH1	approach temperature at outlet of EH1 (°C)	10	300	10*
x <sub>12</sub>	DTEH2	approach temperature at outlet of EH2 (°C)	10	300	10*
X <sub>13</sub>	DTSL2	approach temperature at outlet of SL2 (°C)	10	300	10*
X <sub>14</sub>	DTSL3	approach temperature at outlet of SL3 (°C)	10	300	10*
X <sub>15</sub>	DTSL4	approach temperature at outlet of SL4 (°C)	10	300	107
X <sub>16</sub>	DTSM3	approach temperature at outlet of SM3 (°C)	10	300	252.9
X <sub>17</sub>	DTSM4	approach temperature at outlet of SM4 (°C)	10	300	10*
X <sub>18</sub>	DTSH4	approach temperature at outlet of SH4 (°C)	10	300	10*
X <sub>19</sub>	DTSR4	approach temperature at outlet of SR4 (°C)	10	300	10*

Table.8 Variables for Best Solution Found

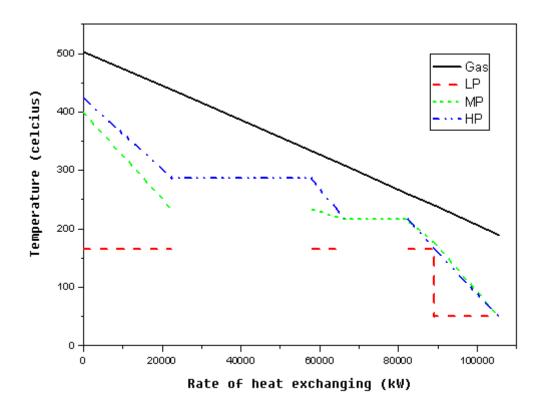


Figure.41 a Compromise between high efficiency and low cost

Figure 41 indicates that seeking the best thermoeconomical ratio forces a compromise between high efficiency and low cost resulting in an increase of about 100°C in exhausted gas temperature of the HRSG. In addition, as the solution gets better and better, the mass flow of low pressure steam approaches zero. This implies that the three-pressure HRSG system should be discarded in favor of a two-pressure HRSG system like that depicted in Figure 42. This will dramatically reduce the complexities that must be considered. This result is consistent with current practice where it is usual that level gas turbine combined cycle systems use two-pressure HRSG systems.

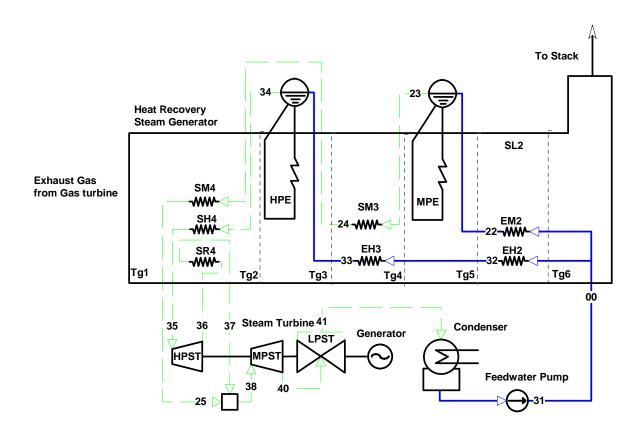


Figure.42 Two pressure configuration

	Name	Meaning of variables	Lower	Upper	Optimum
			Bound	Bound	
<b>x</b> <sub>1</sub>	PLP	pressure of low pressure evaporator (bar)	3	20	10.0
<b>X</b> <sub>2</sub>	PMP	pressure of middle pressure evaporator (bar)	20	60	22.5
X <sub>3</sub>	PHP	pressure of high pressure evaporator (bar)	60	200	103.3
X <sub>4</sub>	DTAL	sub cool temperature of low pressure water (°C)	3	-	127.5
X <sub>5</sub>	DTAM	sub cool temperature of middle pressure water (°C)	3	-	7.6
X <sub>6</sub>	DTAH	sub cool temperature of high pressure water (°C)	3	-	3.0*
X <sub>7</sub>	DTPL	pinch temperature of low pressure stream (°C)	3	-	63.0
x <sub>8</sub>	DTPM	pinch temperature of middle pressure stream (°C)	3	-	33.0
X9	DTPH	pinch temperature of high pressure stream (°C)	3	-	47.2
X <sub>10</sub>	DTEM1	approach temperature at outlet of EM1 (°C)	10	300	42.6
X <sub>11</sub>	DTEH1	approach temperature at outlet of EH1 (°C)	10	300	47.6
X <sub>12</sub>	DTEH2	approach temperature at outlet of EH2 (°C)	10	300	32.6
X <sub>13</sub>	DTSL2	approach temperature at outlet of SL2 (°C)	10	300	69.6
X <sub>14</sub>	DTSL3	approach temperature at outlet of SL3 (°C)	10	300	160.5
X <sub>15</sub>	DTSL4	approach temperature at outlet of SL4 (°C)	10	300	290.5
X <sub>16</sub>	DTSM3	approach temperature at outlet of SM3 (°C)	10	300	80.1
X <sub>17</sub>	DTSM4	approach temperature at outlet of SM4 (°C)	10	300	86.1
X <sub>18</sub>	DTSH4	approach temperature at outlet of SH4 (°C)	10	300	66.9
X <sub>19</sub>	DTSR4	pressure of low pressure evaporator (bar)	10	300	96.0

Table.9 Optimum variables for Thermo-economical ratio

Table.9 presents the best found solution for thermoeconomical ratio problem. In this solution, only two variables are close to their low bounds. The remaining 17 variables values reside in the middle of their limits. From Figure 42, it can be seen that the TS-DPS algorithm works well, converging in 80s cpu time when we use a composite

neighborhood direct pattern search methodology with a one variable deterministic neighborhood (1-VDNB) plus a two variable deterministic neighborhood (2-VDNB).

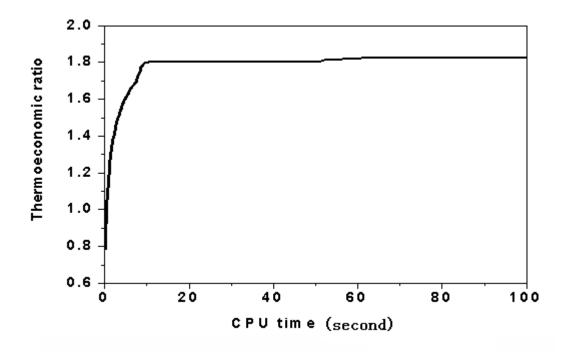


Figure.43 Convergence of thermoeconomic ratio

## 5.3 Effect of neighborhood definition

We tested the three-pressure HRSG problem using different neighborhood definitions and compared their process of convergence. The results are presented in Figure 43. The composite deterministic neighborhood definition with one variable perturbing and two variables perturbing (1-VDNB + 2-VDNB) produces the largest objective function value.

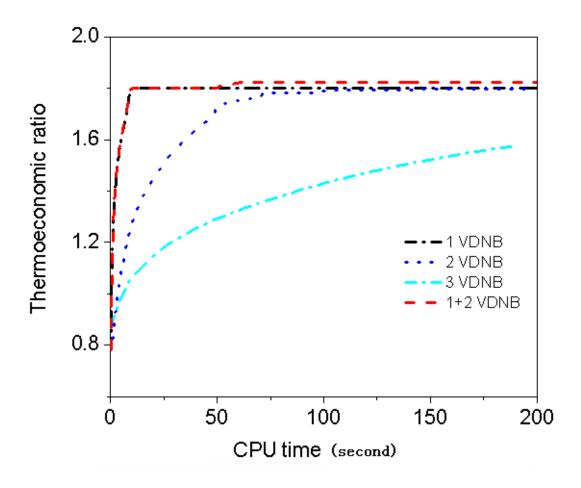


Figure.44 Effect of neighborhood definitions

## **Chapter 6: Conclusions**

We have developed a hybrid global algorithm combining TS and coordinate direct pattern search. We used a *deterministic* variable perturbing neighborhood definition with dynamic step size which is markedly different from the random neighborhood definition that appeared in previous research. Our neighborhood definition extended ideas from coordinate direct pattern search to take better advantage of the local convexity information of a smooth continuous objective function for engineering problems in which the variables have special physical meanings. To exploit continuous function step size sensitivities of different variables, we used TS to save memory efficiently and adjust the discretization step size dynamically to hasten convergence.

In this report, we show that TS algorithm can be successfully applied to optimize a three pressure level HRSG system with continuous 19 independent variables and continuous objective functions. We believe that this TS based algorithm can be successfully applied to a wide variety of additional engineering problems where no derivative information is available.

## References

- L. Attala, B. Facchini, G. Ferrara, (2001). Thermoeconomic optimization methods as design tool in gas-steam combined plant realization, Energy Conversion and Management 42 (2001) 2163-2172.
- Alessandro Franco, Alessandro Russo, (2002). Combined cycle plant efficiency increase based on the optimization of the heat recovery steam generator operating parameters, International Journal of Thermal Sciences 41 (2002) 843–859.
- Manuel Valdes, M. Dolores Duran, Antonio Rovira, (2003). Thermoeconomic optimization of combined cycle gas turbine power plants using Genetic algorithms, Applied Thermal Engineering 23 (2003) 2169-2182.
- Manuel Valdes, Antonio Rovira, M. Dolores Duran, (2004). Influence of the heat recovery steam generator design parameter on the Thermoeconomic performances of combined cycle gas turbine power plants, International Journal of Energy Research, 2004; 28:1243-1254.
- Glover, F. and laguna, M. Tabu Search, (1993). In modern heuristic techniques for combinatorial problem, C. R. Reeves(ed.). Blackwell, Oxford. 70-150
- Harwig, J. Barnes, J.W., More, J., (2001). An Adaptive Tabu Search approach for 2-dimensional orthogonal packing problems, technical report 04-01, the graduate program in Operations Research and Industrial Engineering, The University of Texas of Austin, Austin, Texas.
- Carlton, W. and Barnes, J. W. (1996). Solving the Traveling Salesman Problem with time windows using Tabu Search, Institute of Industrial Engineering Transactions 28: 671-729.
- Battiti, R. and G. Tecchilolli., (1994). The Reactive Tabu Search, Operations Research, Journal on Computing, 1994, 6:2, 126-140.
- B. Colletti, J. W. Barnes and S. Dokov, (1999). A Note on Characterizing the k-Opt Neighborhood via Group Theory, Journal of Heuristics, 5, 1999.
- J. W. Barnes, V. Wiley, J. Moore, and D. Ryer, (2004). Solving the Aerial Fleet Refueling Problem using Group Theoretic Tabu Search, 2004, Mathematical and Computer Modeling, 6-8.
- Margaret H. Wright, (1995). Direct search methods: Once scorned, now respectable, Proceedings of the 1995 Dundee Biennial Conference in Numerical Analysis). 191-208, Addison Wesley Longman, Harlow, United Kingdom.

- J.A. Nelder, R. Mead, (1965). A simplex method for function minimization, The Computer Journal 7 (1965) 308–313.
- K.I.M. Mckinnon, (1998). Convergence of the Nelder-Mead Simplex method to a nonstationary point, SIAM, J. OPTIM, 1998, Vol. 9, No. 1, 148-158.
- Tamara G. Kolda, Robert M. Lweis and Virginia Torczon, (2003). Optimization by Direct search: new perspective on some classical and modern methods, SIAM Review, 2003, Vol. 45 No.3 pp385-482
- N. Hu, (1992). Tabu Search method with random moves for globally optimal design, Int. J. numerical methods eng., 35, 1055-1070 (1992).
- P. Siarry, G. Berthiau, (1997). Fitting of Tabu Search to optimize functions of continuous variables, International Journal for Numerical Methods in Engineering 40 (1997) 2449–2457.
- Rachid Chelouah, Patrick Siarry, (2005). A hybrid method combined continuous Tabu Search and Nelder-Mead simplex algorithms for the global optimization of multiminima functions, 2005, European Journal of Operational Research 161, 636-654.
- Rachid Chelouah and Patrick Siarry, (2000). Tabu Search applied to global optimization, European Journal of Operational Research, Volume 123, Issue 2, 1 June 2000, Pages 256-270.
- G. E. P. Box (1957). Evolutionary operation: a method for increasing industrial productivity. Applied Statistics, Issue 6, Pages 81-101.
- R. Hooke and T. A. Jeeves (1961). 'Direct search' solution of numerical and statistical problems. Journal of the Association for Computing Machinery, 8:212-229.
- B. Lin, D. C. Miller, (2004). Tabu search algorithm for chemical process optimization, Computers and Chemical Engineering 28 (2004) 2287–2306.
- Magnus C. Rydstrand\_, Mats O. Westermark, Michael A. Bartlett, (2004). An analysis of the efficiency and economy of humidified gas turbines in district heating applications, Energy 29 (2004) 1945–1961
- Dimitri P. Bertsekas, (2003). Nonlinear Programming, second edition.
- J. W. Barnes, Dokov, S., Dimova, B., and Solomon, A., (2003). A Theory of Elementary Landscapes, Applied Mathematics Letters, 16, 2003.
- Neil Petchers. (2003). Combined heating, cooling & power handbook: technologies & applications: an integrated approach to energy resource optimization.
- Ramesh K. Shah, Dusan P. Sekulic. (2003). Fundamentals of heat exchanger design.
- V. Ganapathy. (2003). Industrial boilers and heat recovery steam generators: design, applications, and calculations.

- V. Ganapathy, (1993). Steam plant calculations manual.
- Meherwan P. Boyce, (2002). Handbook for cogeneration and combined cycle power plants.
- Rolf Kehlhofer et al. (2009). Combined-cycle gas & steam turbine power plants.
- Francesco Franze and Nicola Speciale, (2001). A tabu-search-based algorithm for continuous multiminima problems, Int. J. Numer. Meth. Engng 2001; 50:665-680.
- P. Siarry, g. Berthiau, (1997). Fitting of tabu search to optimize functions of continuous variables, International journal for numerical methods in engineering, vol. 40, 2449-2457 (1997)
- Y.S. Teh, G.P. Rangaiah, (2003). Tabu search for global optimization of continuous functions with application to phase equilibrium calculations, Computers and Chemical Engineering 27 (2003) 1665-1679
- Aspelund, T. Gundersen, J. Myklebust, M.P. Nowak, A. Tomasgard, (2009). An optimization-simulation model for a simple LNG process, Computers and Chemical Engineering, 2009
- Eylem Tekin and Ihsan Sabuncuoglu, (2004). Simulation optimization: A comprehensive review on theoryand applications, IIE Transactions (2004) 36, 1067–1081
- José M. Ponce-Ortega, Medardo Serna-González, Arturo Jiménez-Gutiérrez, Use of genetic algorithms for the optimal design of shell-and-tube heat exchangers, 2009
- Antonio Rovira, Manuel Valdés and Jesús Casanova, A new methodology to solve nonlinear equation systems using genetic algorithms. Application to combined cycle gas turbine simulation, 2005
- M. Mohagheghi, J. Shayegan, Thermodynamic optimization of design variables and heat exchangers layout in HRSGs for CCGT, using genetic algorithm, 2009
- José M. Ponce-Ortega, Medardo Serna-González, Arturo Jiménez-Gutiérrez, (2009). Use of genetic algorithms for the optimal design of shell-and-tube heat exchangers, Applied Thermal Engineering 29 (2009) 203–209
- Mehdi Mehrpooya, Farhad Gharagheizi, Ali Vatani, (2006). An Optimization of Capital and Operating Alternatives in a NGL Recovery Unit, 2006, Chem. Eng. Technol. 2006, 29, No. 12, 1469–1480
- Won-Hyouk Jang, Juergen Hahn, Kenneth R. Hall, (2005). Genetic/quadratic search algorithm for plant economic optimizations using a process simulator, Computers and Chemical Engineering 30 (2005) 285–294
- Robert Michael Lewisa, Virginia Torczona, Michael W. Trossetc, (2000). Direct search methods: then and now, Journal of Computational and Applied Mathematics 124 (2000) 191-207

- Lars Magnus Hvattum, Fred Glover, (2009). Finding local optima of high-dimensional functions using direct search methods, 2009, European Journal of Operational Research 195 (2009) 31–45
- Marco A. Luersen, Rodolphe Le Riche, Globalized Nelder–Mead method for engineering optimization, 2004, Computers and Structures 82 (2004) 2251–2260
- Rachid Chelouah, Patrick Siarry, Genetic and Nelder–Mead algorithms hybridized for a more accurate global optimization of continuous multiminima functions, European Journal of Operational Research 148 (2003) 335–348
- L. C. W. Dixon and G. P. Szego (eds.). (1978). Towards Global Optimization 2, North-Holland, Amsterdam, 1978.
- K. Schittkowski and W. Hock, (1987). More test examples for nonlinear programming codes, Lecture Notes in Economics and Mathematical Systems, Vol. 282, Springer, Berlin, 1987.

Aspen Plus User Guide, Version 10.2, (2000)

Aspen Plus User Guide, Version (2006)

Ryan Reid, (2008), a Study in the Benefits of Efficiency Improvements to Emissions and Fuel Costs. http://www.utexas.edu/utilities/sustainability/

Vita

Zelong Liu was born in Heilongjiang province, P.R. of China on December 1965,

the son of Liangsheng Liu and Shuqin Li. He graduated from the Nehe First High School,

Qiqihaer city, Heilongjiang province, P. R. China, in 1984 and was admitted to the

Tsinghua University in Beijing, P. R. China. He received a degree of Bachelor of

Engineering from the Department of Mechanics in 1989, and was admitted to the

graduate program of the Institute of Engineering of Thermophysics, Chinese Academy of

Sciences. At spring of 1992, he received a Master of Science in Mechanical Engineering

He then took a position with the Chinese National Search Laboratory as a researcher

where he conducted energy power generation system simulation and optimization

research and performed consulting tasks with industrial concerns. He was awarded

several projects as a Principle Investigators from the Chinese National Science

Foundation and the State Power Corporation of China. In the September of 2004, he

entered the graduate program of the Operations Research and Industrial Engineering at

the University of Texas at Austin. Started from July of 2006, he worked for the Alcoa

global purchasing department at San Antonio as an operations analyst, for the Entek

Manufacturing Inc. at San Antonio as a design/project engineer, and for the Alliance

Structural Engineers LLC at Houston as a design engineer/business analyst.

Permanent address: 5001 Convict Hill Rd, Apt. 402, Austin TX 78749

This report was typed by author.

72