Artificial Invention:
Synthesis of Innovative Thermal Networks, Power Cycles, Process Flowsheets and Other Systems

by

Alexander Kott

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FOREWORD
TO THE 2005 PUBLICATION

The content of this volume is my doctoral dissertation originally titled *Automated Synthesis of Thermal Systems Using Heuristic Search and Exergy Analysis*. The research behind this work won the E. F. Qbert Outstanding Paper Award of the American Society of Mechanical Engineers. The award statement spoke of "innovative research," and I thought the word innovative was particularly fitting. Indeed, the key motivation behind this work was the quest for a computational method that could produce innovative designs of systems: not merely an optimization of numerical parameters of a known system concept but rather a synthesis of novel combination of components. The goal of this book is to introduce a computational method that comes surprisingly close to a process of invention. Hence the new title of this edition, *Artificial Invention.*

The proposed approach touches on several well-defined fields of study, including flowsheet synthesis, design of power cycles, liquefaction and refrigeration systems, and heat exchange networks. It also introduces a generalization and extension of the technique called pinch technology. However, the most significant contribution of this work is the systematic computational approach to innovative design of engineered artifacts in general, not only thermal and power systems. It demonstrates that transformational approach to design can yield design concepts comparable to human inventions.

The main ideas of this approach have been implemented in a computer program called TED, which invents conceptual schematics of optimized thermal systems (the name of the program is a loose acronym of Thermal Energy systems Designer). TED is an inventor of its systems in the sense that it generates the structure (topology) of the system "from scratch." It does not merely optimize numerical parameters (e.g., flows or pressures) for a given topology, for TED is not given the topology of the system. Nor does TED select and combine predefined and stored systems or cycles, for it does not have a library of known systems and cycles. Nor does TED arrive to its result by pruning some predefined generalized topology, for it does not assume any.

Invention, whether artificial or human, is rooted in exploration. A key claim of this work is that innovative design can be modeled as a search process using elements of search algorithms that originated in the field of Artificial Intelligence. The synthesis process is modeled as a heuristic search conducted in a state-space of all possible design versions (design states). TED explores one design possibility after another in a systematic fashion, looking for a solution to the design requirements.

Invention, however, is not an unguided exploration. Because TED specializes in invention of thermal systems, it evaluates each design state using a special technique of exergy analysis applied to an infinitesimal temperature interval. This allows one to describe the thermal system by several integral characteristics which are functions of temperature. A particularly important integral characteristic – a measure of system's Second Law infeasibility – is introduced in this work; it allows a uniform treatment of both feasible and infeasible design states. The method of exergetic analysis used by TED utilizes (and possibly – subsumes) ideas of the pinch technology. Artificial invention systems that specialize in systems other than thermal would require other domain-specific techniques for evaluating design states.

An invention process cannot succeed unless the inventor's exploration is combined with learning. This work introduces a particular form of learning and demonstrates its crucial importance to the effective exploration of the design space. Every design state, except for the initial state, has a parent state from which it was produced. If the newly produced child state is worse (i.e., has lower likelihood of leading to a desired solution) than its parent, TED grows more skeptical about the potential of the parent state and reduces its expectations regarding this branch of the design space. Then the same is done with the grandparent, and so on. This reevaluation of parents based on the behavior of their descendants is a form of learning based on backpropagation. By learning to be skeptical about less promising design approaches, the artificial inventor guides itself toward a successful invention.

Ultimately, the proof of inventor is in inventions. In this volume, the reader finds several examples and step by step traces of the process by which TED invents a number of sophisticated and thermodynamically advanced system designs that would be non-trivial to generate by other means. Some of these inventions do not follow any particular known classic cycles or system concepts; these are TED's own creations. In other cases TED rediscovered at least two significant and well known inventions: the Linde Dual-pressure system and the Claude system. Then TED continued to optimize one of these schemes and arrived at a somewhat more sophisticated and efficient system.

Some would argue that the term artificial invention is an oxymoron, and that a machine-made invention is, in some fundamental way, preconceived by the machine's creator and therefore cannot be truly innovative. Whether or not such objections are valid, tools like TED can evolve into powerful practical tools that would assist human inventors. And if the objections are valid, I am satisfied that this work encourages important questions about the very nature of human creativity and inventiveness.

ACKNOWLEDGMENTS

I am deeply indebted to the co-advisors of this thesis - Dr. Charles C Hwang and Dr. Jerrold H. May. Dr. Hwang provided overall management of the project and guided the Mechanical Engineering aspects of the research. Dr. May's contributions made possible those directions of the thesis that touch on the techniques of Artificial Intelligence. In 1986, when I first approached both of them with the proposal to commence this project, the proposal consisted of little more than ambitious plans and vague concepts. Without their insight, trust, and encouragement, those timid beginnings would never have developed into a dissertation.

Digital Equipment Corporation provided a generous grant that allowed me to quit my full-time job and to spend a year working on this research at the Department of Mechanical Engineering of the University of Pittsburgh. I wish to say that it was one of the most enjoyable and productive years of my life. It is doubtful that the project could ever have been completed without this financial support.

For three other years my time was divided between this thesis and a full-time engineering work. This would not be possible without the help and good will of my supervisors. Ron Aungier of Elliott Turbomachinery Company and Allan Tomalesky of Carnegie Group, Inc. have been most supportive and appreciative of my efforts to further my academic background.

Professor Michael J. Moran and Ms. Rita A. Bajura of the DOE Morgantown Energy Technology Center became involved in this research at a relatively early stage, when I submitted some preliminary results to the 1987 Winter Annual Meeting of the American Society of Mechanical Engineers. Their valuable comments, criticism, and suggestions helped that submission win the E. F. Qbert Outstanding Paper Award. It was a major encouragement, for which I am grateful to all members of the ASME Advanced Energy Systems Division.

Finally, special thanks to those dear ones whose contributions I cannot even begin to acknowledge -my parents, my wife, my children, and my friends. Thanks for all your efforts, patience, forgiveness, and love.

ABSTRACT

This dissertation proposes a computational technique for automated "invention" of conceptual schemes of thermal systems. The input provided to the automated problem solver is a description of the streams entering and leaving the system. The output is a network of elementary processes: compression, expansion, heating, cooling, and chemical processes. The problem solver seeks a network that is feasible, and offers an optimal (or at least favorable) combination of energy and capital costs. The synthesis process is modeled as a heuristic search conducted in a state-space of all possible design versions. The main ideas of the dissertation have been implemented in a computer program called TED, which invented a number of nontrivial schemes.

TED starts with an initial state (or states), which may be either proposed by the user or generated automatically. TED evaluates each state using a special technique of exergy analysis applied to an infinitesimal temperature interval. This allows us to describe the thermal system by several integral characteristics which are functions of temperature. One particularly important integral characteristic - a measure of system's Second Law infeasibility - is introduced in this work; it allows a uniform treatment of both feasible and infeasible design states.

TED then selects the most promising of the available designs. This selection is guided by a specialized search algorithm BP* which is shown to be probabilistically admissible. The results of the exergy analysis are used to perform a look-ahead evaluation of the design states. BP* also uses backpropagation of the state evaluation function to reduce the amount of backtracking.

TED then improves the selected design by applying one of the transforming operators and thereby generating a new design. Each transformation involves addition of an incremental network of thermal processes to the original state and reduces either irreversibility (exergy loss) or infeasibility of the thermal system. The application of the transformations is controlled by a heuristic move generation function that selects the most promising transformations. The new design is added to the database of the available design states.

The search continues with these evaluate-select-transform iterations until an (approximately) optimal design is found.

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NOMENCLATURE

Symbol	Explanation
'	indicates (1) differentiation in respect to time, or (2) modified or different system or state
A	a set of components available for constructing the system
A*	a heuristic search algorithm proposed by Hart, Nilsson, and Raphael
BP*	a heuristic search algorithm proposed in this dissertation
c_i	a constraint
$compr$	refers to a compression process
C	a set of constraints
C_c	the current cost of a design state
C_d	the direct cost of a design state
C_{eq}	the annualized cost associated with system's equipment
C_h	the cost of heat, Appendix A
C_p	the heat capacity at constant pressure
C_{pu}	the annual cost of power and utilities consumed by the system
$C_{pu,n}$	the non-recoverable part of cost C_{pu}
$C_{n,best}$	the projected cost of the best goal state reachable from a given state
$C_{n,bp}$	the projected cost of a state after the backpropagation process
C_v	penalty (expressed as annual cost) for violation of constraints
C_Λ	a penalty (cost) for the system's Second Law infeasibility
$CLOSED$	a list of expanded states
e	exergy, on a molal basis
e^0	standard state exergy, on a molal basis
e_{lim}	a value of exergy defined in respect to the limiting temperatures of a process (Chapter 4)
$expan$	refers to an expansion process
E	exergy
E	a set of relations among the design elements
E^0	standard state exergy

f	a heuristic evaluation or cost function
f_L	a function that evaluates influence of the state's irreversibility on the state's projected cost
f_Λ	a function that evaluates influence of the state's infeasibility on the state's projected cost
final	refers to the final conditions of a process
f'	a heuristic backpropagated cost function
F	a set of feasibility constraints in an equipment-level problem
F'	a set of feasibility constraints in a process-level problem
$F^h(T)$	enthalpy flux
$F^e(T)$	the exergy flux
g	a cost function or a current cost function
G	a set of infeasibility constraints in an equipment-level problem
G'	a set of infeasibility constraints in a process-level problem
GDP	the General Design Problem
GTND	the General Thermal Network Design Problem
h	enthalpy, on a molal basis
h	a function that estimates additional cost required to reach a goal state
h^0	standard state enthalpy, on a molal basis
h_0	enthalpy at environmental conditions, on a molal basis
h_{lim}	a value of enthalpy defined in respect to the limiting temperatures of a process (Chapter 4)
H^+	a transforming operator, a type of transformation
H^-	a transforming operator, a type of transformation
i	subscript indicates reference to different material streams, or different chemical substances within a given stream
i	a set of components found within the system
in	subscript indicates entrance condition or direction
initial	refers to the initial conditions of a process
is	refers to an isentropic process
j	subscript indicates reference to different material streams, or different chemical substances within a given stream
k	subscript indicates reference to different material streams, or different chemical substances within a given stream
k	a coupling recipe that defines interactions between the system's components

k_L	the coefficient in the linearized form of f_L, a unit cost of irreversibility
k_Λ	the coefficient in the linearized form of f_Λ, a unit cost of infeasibility
L	exergy loss, irreversibility
Lisp	a computer language used to implement a computer program for this research
m'	the mass flow rate of a process
match-by	a process of the incremental network that is to be merged with a process of the existing network
match-to	a process of the existing network (parent state) that is to be merged with a process of the incremental network
n	number of moles
n	a multiplier that indicates direction of the process (Chapter 4)
n	a state in a search problem
n'	a child state of state n
N	a network of elementary thermal processes
N	a positive integer
NP-hard	a property of a problem, Appendix A
out	subscript indicates exit condition or direction
OPEN	a list of unexpanded states
p	a penalty associated with a design element
P	pressure
P	total penalty function (cost) of a system in an equipment-level problem
P	probability
P'	total penalty function (cost) of a system in a process-level problem
P^+	a transforming operator, a type of transformation
P^-	a transforming operator, a type of transformation
P_i	the probability that child i leads toward the best goal state
$P_{s\text{-}\gamma}$	a path from state s to state γ
Q	heat
$Q(T)$	the heat transit function of a system
R^+	a transforming operator, a type of transformation
R^-	a transforming operator, a type of transformation
RP^+	a transforming operator, a type of transformation
RP^-	a transforming operator, a type of transformation

s	entropy, on a molal basis
s	an initial state in a search problem
s	a size of a design element
s^0	standard state entropy, on a molal basis
s_0	entropy at environmental conditions, on a molal basis
S	a design state
S'	a child state of S or any state different from S
SDP	the Specific Design Problem
S	entropy
S^*	the optimum network of elementary processes, a solution of the process-level synthesis problem
t	a transformation
T	temperature
TED	Thermal Designer, an experimental program that implements ideas of this dissertation
T_{low}	the lowest temperature of an incremental loop
T_{high}	the highest temperature of an incremental loop
T_{mid}	the intermediate temperature of an incremental loop
T_{max}	the maximum temperature of a system or of a process
T_{min}	the minimum temperature of a system or of a process
T^0	the standard state temperature
T_0	environmental temperature, "dead state" temperature
T_1	the lower bound of a temperature interval or any fixed temperature value
T_2	the higher bound of a temperature interval
v	a design element
v	a stoichiometric coefficient
V	a set of design elements
W	work
$W(T)$	the work function of a system
X	inputs and outputs of a system in an equipment-level problem
X	costs that cannot be explicitly minimized by the available set of transformations
X'	inputs and outputs of a system in a process-level problem
X^*	definition of the system's inputs and outputs

Y	costs that can be explicitly minimized by the available set of transformations
Z	a system
Z	heat of reaction
$Z(T)$	the heat of reaction function of a system
Z^+	a set of natural numbers
Z^*	a network of equipment units that corresponds to S^*
γ	a goal state in a search problem
δ	a bound on probability value
δ	a change in the value of a parameter that results from applying a transformation, a difference between the parent's parameter value and the child's parameter value
Δ	finite change in a value of a parameter
ΔN	an incremental network of elementary thermal processes
Δn	the extent of reaction, change in molal composition
η	efficiency of a work exchange process or a combined efficiency for a set of work exchange processes
Λ	exergy creation, Second Law infeasibility measure
μ	chemical potential, on a molal basis
μ^0	standard state chemical potential, on a molal basis
μ_0	chemical potential at environmental conditions, on a molal basis

1.0 INTRODUCTION

1.1 The Problem

This dissertation focuses on the synthesis of conceptual schemes of thermal systems. Examples of such systems include gas turbine engines, thermal environmental control systems, steam power plants, chemical processes, refrigeration, and liquefaction plants.

Consider the design problem illustrated in Figure 1. In this particular case, we wish to design a system which has three ***inputs***, streams of some gases, and three ***outputs***, streams of the same gases, but at different pressures and temperatures. The system is supposed to accomplish the transformation of the input streams into the output streams. The internals of the system are not known - they are to be designed. As shown in the figure, there are also several cooling and heating ***utilities*** - material streams that can be used to absorb or to provide heat, e.g., a cooling water - defined in this problem. Which utilities will be used and in what quantities is not known either. Definitions of inputs, outputs, and utilities are the major elements of the system ***specification***.

Given the specification, we wish to design a ***conceptual scheme*** of the system. The conceptual scheme should consists of some number of basic ***processes***, such as cooling, heating, compression, expansion, and chemical reactions. An example of such a conceptual scheme is shown in Figure 2. This scheme is one possible solution to the above problem. Each of the three streams goes through a number of heatings, coolings, expansions and compressions. There are also some recycles - flow patterns where a stream is split into two streams and one of the two is merged with the original stream at some point upstream of the splitting point. The streams exchange heat among themselves and with some of the utilities. There is also some production and exchange of mechanical power. Notice that the conventional representation of a power or refrigeration cycle, e.g., a T-S diagram description of a Rankine cycle or of a Claude cycle, can be viewed as a special case of the conceptual scheme.

As in any design problem, the system must be ***feasible***, i.e., it must satisfy a number of applicable

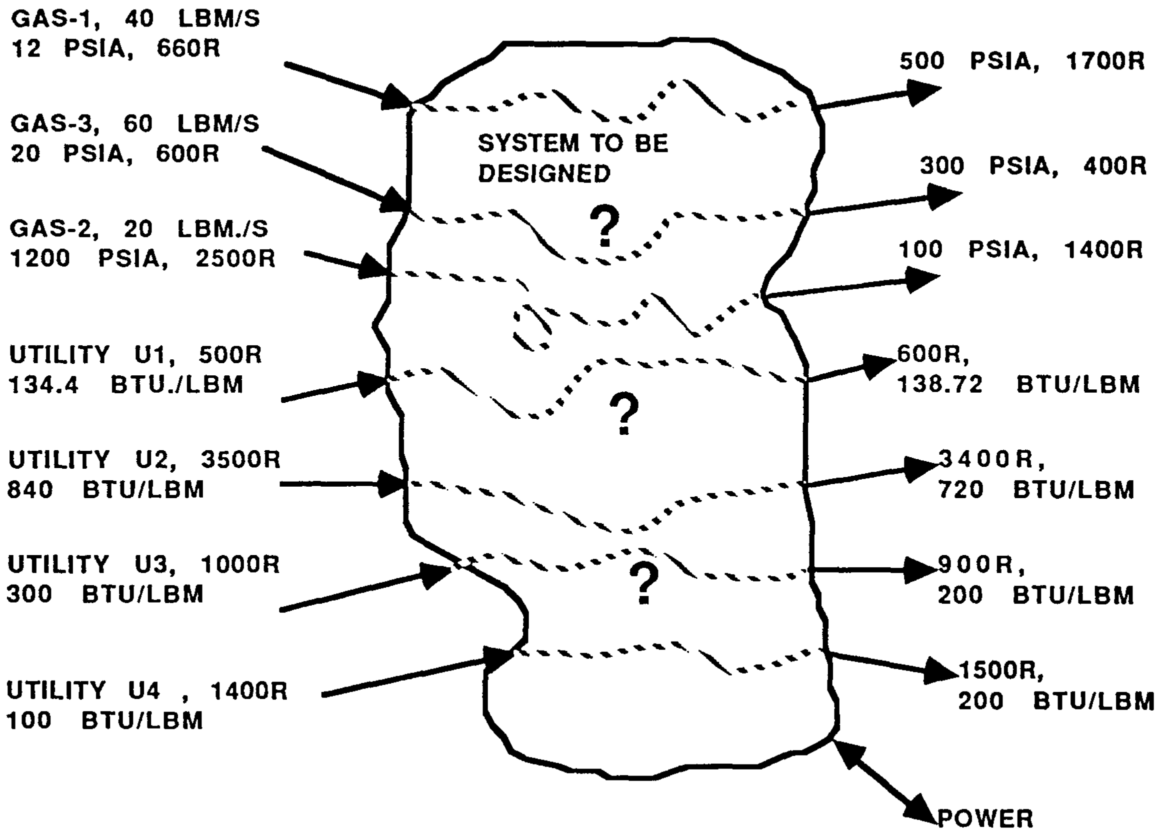

Figure 1. An example of a thermal system design problem.

constraints. It must comply with the known physical laws, particularly with the Laws of Thermodynamics. It must also be consistent with the intended equipment technology, e.g., maximum temperatures and pressures allowable in the heat exchangers. Besides the constraints, we must also be concerned with the system's ***overall cost***, which should in some way account for the cost of system's machinery, cost (or income form the sale) of utilities and power, and other costs. Ideally, we would like to find an ***optimum*** system - the one that has the lowest possible overall cost. In practice, however, we may often find it necessary to relax the optimality requirement and accept a solution that is merely "reasonably good."

The example above is fairly simple. In a more general case, we may expect a large number of inputs/outputs. The streams may split, mix and react with each other. The chemical composition of the output streams may not be the same as that of the input streams, etc. In some cases, the system specification

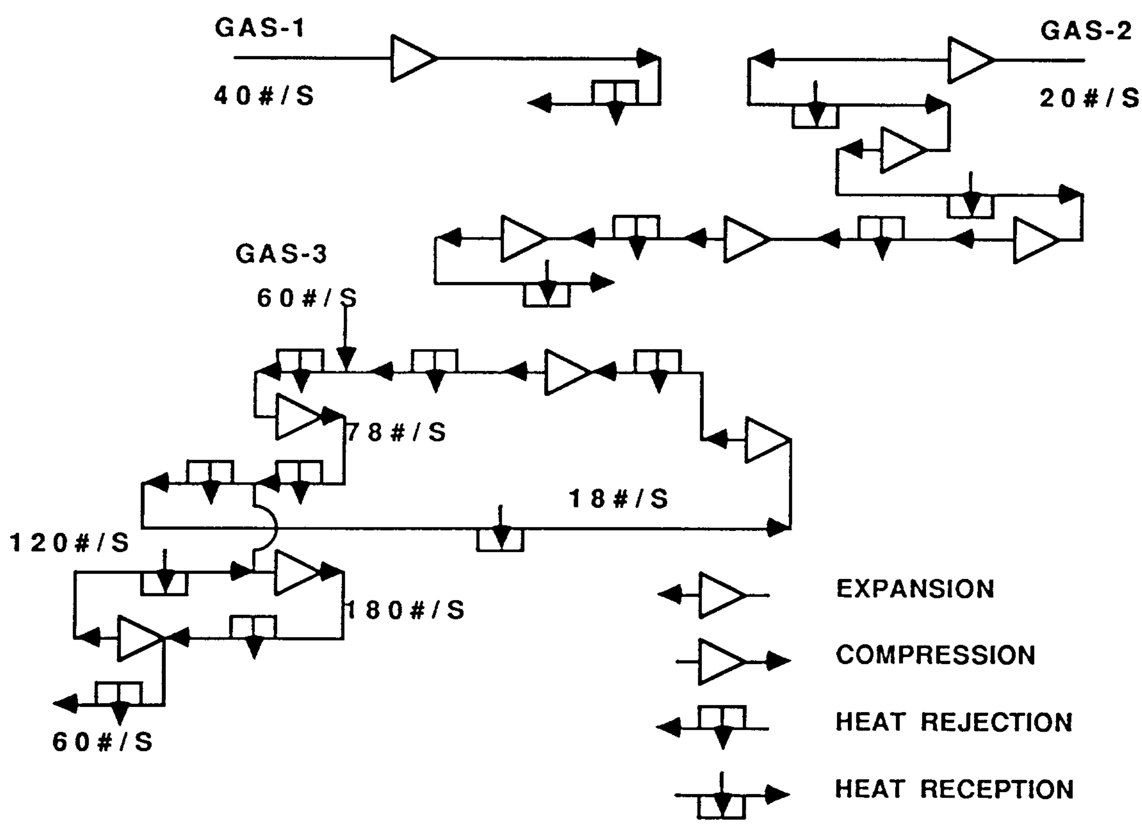

Figure 2. A conceptual scheme* (a network of elementary processes) which is one possible solution to the problem in previous figure.

may include an initial conceptual scheme, which may be neither optimal nor feasible; then the problem solver is required to improve upon the initial design. In case of a closed system, when there are no material inputs/outputs, the system specification may include the required cooling and heating loads, the power usage/production requirements, and the initial scheme.

The computational complexity of the problem is formidable. Like many other design problems, this problem is NP-hard. The number of possible conceptual schemes for such a system is infinite or extremely large. The thermodynamic and economic effectiveness of different alternatives may vary widely, depending on the trade-offs between the equipment-related costs, opportunities to integrate heat-exchange processes, and other factors.

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*Section 9.1 explains graphic representations used in this dissertations