An Algorithm for Control Volume Analysis of Cryogenic Systems

by

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Abstract

This thesis presents an algorithm suitable for numerical analysis of cryogenic refrigeration systems. The need for such an algorithm arises from the absence of effective analysis tools in the cryogenic field.

Typically, preliminary design of a cryogenic system commences with a number of decoupling assumptions with regard to the process variables of heat and work transfer (e.g. work input rate, heat loading rates) and state variables (pinch points, momentum losses). These assumptions are made to facilitate direct and simplified solution calculations. However, making preliminary performance estimations minimizes the effect of component interactions which is inconsistent with the intent of "analysis". A more useful design and analysis tool is one in which no restrictions are applied to the system - interactions become absolutely coupled and governed by the equilibrium state variables. Such a model would require consideration of hardware specifications and performance data and information with respect to the thermal environment. Model output would consist of the independent thermodynamic state variables from which process variables and performance parameters may be computed. This model will have a framework compatible for numerical solution on a digital computer so that it may be interfaced with graphic symbology for user interaction.

This algorithm approaches cryogenic problems in a highly-coupled state-dependent manner. The framework for this algorithm revolves around the revolutionary thermodynamic solution technique for Computer Aided Thermodynamics (CAT), developed by Dr. Gilberto Russo at the Massachusetts Institute of Technology. Fundamental differences exist between the Control Volume (CV) algorithm and CAT, which will be discussed where appropriate.

This thesis presents the algorithm in detail with respect to the thermodynamic principles, state-variable management, device models, system networking, solution structure, numerical reduction, model flexibility and generality and potential pitfalls.

Thesis Supervisor: Professor Joseph L. Smith, JR.
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For my shipmates, who rest in peace.

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I owe many debts in the formulation of this thesis. I am especially grateful to Professor Smith under whose tutilage I garnered much knowledge I may have never found elsewhere. He was most helpful in lending direction where there seemed to be none and perspective when it was lost.

I must express sincere gratitude to Dr. Gilberto Russo, who lectured me with great patience until I grasped the salient points of Computer Aided Thermodynamics. He was selfless in his assistance and was my principal consultant as I waded through the algebraic, thermodynamic and numerical details; he shared many of my headaches.

I would also like to thank Doctors Alan Kornhauser, Jim Chafe and Alan Crunkleton, all graduates of the Cryogenic Engineering Laboratory who lended much blackboard advice.

Certainly, I cannot say enough about my wife, Jennifer, who had the ability to soothe my apprehension and anxiety throughout this work while she actively pursued her own professional aspirations.

Finally, I would like to express my gratitude to the United States Navy for giving me the opportunity to take my career through MIT, an experience that will remain with me for the remainder of my military and technical career.

Biographical Note

Michael Brian Stanton [redacted] lived and graduated secondary school in 1979.

In 1983, he was a distinguished graduate of the U.S. Naval Academy and was commissioned Ensign. After attending naval warfare and engineering schools in Newport, Rhode Island, he was assigned to the Engineering Department of USS SCOTT (DDG-995), where he served as main propulsion and auxiliaries assistant. He was qualified as Surface Warfare Officer and Engineering Officer of the Watch.

He came to MIT in June, 1986 where he studied naval construction engineering and mechanical engineering. He is married to [redacted]Stanton of Durham, North Carolina.

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1 Introduction

1.1 Background

Much design work has been done in the cryogenic engineering field and, accordingly, there are numerous design methods that have proven useful. Design, in an engineering context, means to model physical behavior and assign value to problem variables in such a manner as to achieve a desired engineering effect. A "good" design distinguishes itself from a "bad" design by whether or not the variables and parameters were assigned value in an optimal sense. Optimal is relative, but usually implies maximum desired effect at minimal resource cost. Efficiencies and dimensional analysis variables are typical ways in which engineers evaluate the optimization of a particular design. Thus, *good design requires quality optimization.* Quality optimization requires a thorough understanding of the problem variables, or, more succinctly, good analysis.

Analysis means understanding the interactive behavior of the relevant physical variables. This is the reason good design work is supported by a sound foundation of analytical study. Good analysis tools are not in abundance in the cryogenic field, which forms the basis for this study: *to develop an analysis algorithm* suitable for application to cryogenic engineering systems. A typical analysis method for a closed loop thermodynamic system starts with a definition of the physical system in terms of models for devices (turbines, boilers, etc.) and for their interaction with the environment (Q_{in}, W_{out}, T_{RES},etc.) . To determine the system performance, a number of assumptions must be made to reduce the vast number of unknowns. Such assumptions include the thermodynamic state at the at the inlet/outlet of a device (e.g. saturated, superheated, quality), a ratio of relevant pressures ($\Delta P/P$, P_H/P_L), or a temperature change ratio (T_H/T_L, pinch points). The

effect of making these assumptions is to decouple or minimize the interaction of state variables that govern system behavior; the behavioral patterns of the system become locked out.

A robust analysis is one which minimizes global assumptions allowing the process variables to result directly from the highly coupled interaction of equilibrium state variables. The analysis method could be likened to a black box which takes inputs of component specifications and yields as output the value of the system's equilibrium state variables. It is then a simple extension to transform the state variables into more significant performance parameters. Thus system modelling is achieved by allowing the system to operate in its unrestricted condition compatible with the hardware imposed. Optimization (and hence design) becomes a matter of selecting hardware that achieves the best overall system performance, as defined by the designer. The method which is the heart of this paper pursues this strategy.

Analysis is difficult. It requires simultaneous segregation and synthesis of the problem variables to establish process characteristics or system behavior. Many engineers incorrectly use the word *analysis* when referring to *design* calculations. In fact, analysis in its crudest (yet often practiced) form is executed by conducting a series of design calculations with differing input values and observing the output or performance values. This is analogous to the experimenter plotting the results of a run without first calculating the analytical prediction. Such an analysis method does the segregation while loosing sight of the synthesis. This type of investigation is more appropriately termed *design analysis*.

1.2 Basis for Method

In this work, the methodology for analysis of a thermodynamic system consists of idealization of the physical problem, generation of the mathematics modelling the problem, solution of the mathematical representation and interpretation of the results. The aggregate of these tasks is rather complex. The method presented here reduces the complexity by using simple concepts to construct a complex representation of thermodynamic behavior that will be managed by a computer. This is essentially what is done in a finite element analysis method: building a complex representation to be managed by a computer from almost trivially simple engineering concepts.

The great utility of a digital computer is that it can be programmed to perform the equation(s) generation and mathematical solution (through an intelligent assembly of the "simple parts"), leaving the idealization and interpretation to the user (although some of today's modern routines will assist in the interpretation process by a convenient assembly of the output data). The method to be developed will allow a graphic, symbolic input of the problem, thus further assisting the user in the analysis of alternatives. The ability of a computer to manage large quantities of data (specifically, unknown variables) eliminates the temptation to make decoupling assumptions about problem variables that reduces their number to an (algebraically) manageable level. It is this special feature that makes this method unique: elimination of decoupling assumptions with respect to the problem variables causes the variables to become mathematically unconstrained and therefore physically interactive through the interconnective matching conditions.

In applying a computer to perform thermodynamic analysis, the method employed should be general enough to allow analysis of a wide variety of complex multiple-element

thermodynamic systems. In such an employment, it should use simple models (vis. equation sets) to represent the composite system and the same solution procedure to solve for the requisite data. This was the inspiration behind Computer Aided Thermodynamics (CAT) as developed by Dr. Gilberto Russo at the Massachusetts Institute of Technology. CAT is structurally similar to a finite element analysis except that it is applied to a collection of discrete elements (that may undergo different types of interactions) rather than a homogeneous, continuous system (undergoing a single interaction). The great success of CAT has served as a backdrop for the Control Volume (CV) algorithm: adapting thermodynamic analysis to take advantage of computer power by formulating a new method of analysis.

2 Foundations of Control Volume Method

2.1 Overview

The control volume analysis method is developed for implementation on a digital computer. The basis for the method is modelling of complex systems using simple building elements. These elements come in two broad classifications: storage elements and interconnective elements. Each element has associated with it a set of constitutive relations that describe the element's behavior and are defined in a problem independent manner.

The complete physical system is represented by all the constitutive relations of all the elements making up the system specified for the particular arrangement of elements. Once the elemental constitutive relations become specified for the system (through a change of base or variable transformation), they become the *basis for* the residual relations of the system. *Residual relations* are used to define the steady state behavior of the entire system. The specificity comes from invocation of the *system topology*. The system topology is used to perform the change of base that generates the problem specificity from the "n" sets of constitutive relations of the "n" elements of the mesh. This accomplishes the 'modelling and equation generation' steps in this computer-aided thermodynamic analysis. Solution is found by using the residual functions in a global equilibrium equation:

$$[K'(x_i)]\{\Delta x\} = \{R(x_i)\} \tag{1}$$

$[K'(x)]$ is a matrix of first derivatives of the residual relations $\{R(x_i)\}$ with respect to the independent variables $\{x_i\}$ of the system (i.e. the *Jacobian* matrix). Successive modifica-

tions are made by imcrementing the current value of $\{x\}$ by $\{\Delta x\}$ which will drive $[K^t(x_i)]\{\Delta x\}$ to zero (or less than some appropriate ε). $[K^t(x_i)]\{\Delta x\}=0$ satisfies the constitutive relations of the system. The independent variable vector $\{x_i\}$ for which $\{R(x)\}$ goes numerically close to zero is the equilibrium state of the system and no further increment in x is required.

$[K^t(x_i)]$ is defined as the System Tangent Stiffness Matrix[1]. When $[K^t(x_i)]$ is assigned a numerical value using $\{x_i\}$, $[K^t(x_i)]$ is the linear approximation to the system's residual functions $\{R(x_i)\}$. This linearization is necessary due to the non-linear nature of some of the system's equations. The System Tangent Stiffness Matrix represents an (n-1) dimensional tangent surface to a (n) dimensional function, hence the tag "tangent". The modifier stiffness comes from the congruence between equation (1) and the equilibrium equation for a structural finite element analysis system where the constitutive matrix is often referred to as the "stiffness" matrix.

This paper describes the physical idealization of the thermodynamic problem, generation of the mathematics describing the problem and solution procedure. Interpretation of results is not considered here, since that is a matter of recasting equilibrium state variables into more pragmatic (or new) performance representations (COP, η_{th}, etc.) that may be defined in the post-processing routines.

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1 "A New Methodology of Computer-Aided Thermodynamics", Gilberto Russo [doctoral thesis], Department of Nuclear Engineering, Massachusetts Institute of Technology, January, 1987.

2.2 Compatibility

The algebraic uniqueness and simplicity of each storage element lead one to believe that system simulation is now just a matter of connecting together elements of interest and performing the system integration and reduction. However, the issue of compatibility must be addressed with respect to the interaction of the engineering devices (which are independently defined). In other words, does the 'whole equal the sum of the parts'.

This problem commonly arises during the design of thermal power systems with regard to "matching" of components. For example, does the mass-flow/pressure ratio characteristic of a compressor match that of the turbine it is to operate with? If not, it may be impossible to achieve a steady state operation for the system in the absence of specially designed controls. Such a system (without controls) may oscillate (its performance and state variables) about a stable equilibrium (i.e. hunting), one component may drive the other to operate at an inefficient operating point. The stability of the operating state will require further consideration of the dynamics of the system.

Accordingly, this methodology investigates the steady state operation of systems for which performance parameters (constants or functions) are assigned. Furthermore, the relations and models used to describe component behavior must be consistent with physical limitations of a system. For example, it is incompatible to specify pressure rises for both a compressor and an expander which operate in the same fluid circuit since this would be to over-constrain the problem. Only one pressure ratio can be specified while the other pressure ratio results as a consequence of the interaction of the pressure and mass flow variables in the system. This compatibility is necessary to ensure a steady state can be attained.

To accommodate the compatibility issue during the initial stage of the development of the method, pressure ratios will be defined only for compression devices. All expansion devices (turbines, throttles, etc.) will be void of any pressure characteristic; the equilibrium pressures will be established by the interaction of the system elements.

2.3 Physical Idealization

The physical system is modelled using its constitutive elements . Figure 1 is a representation of a closed loop thermodynamic circuit operating as a refrigeration cycle. While heat and work interactions are an intimate part of the complete operating system, these external interactions are determined after the equilibrium behavior of the system is established. The work or heat interaction for any element is readily determined by simply knowing the inlet and outlet state. This is infact the approach used here: work or heat transfers are determined after the value of the equilibrium state variables are known by writing the 1st Law of thermodynamics in the post processing routines.

The system is the collection of control volumes that contains all components of interest and the environment with which the components interact. A valid thermal analysis of the component interactions can only be done by analyzing a uniquely independent set of control volumes. This system has four distinct components[2]. Accordingly, a set of four independent control volumes must be developed. A selection of any three of the four control volumes shown in Figure 1 plus a control volume encompassing the entire system (including the environment, which is part of the system) is a valid selection. However,

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2 For simplicity in this development, interconnective piping and flow passages are assumed to be lossless. Lossy flow in interconnecting piping may be incorporated into the framework upon extension of the applicable constitutive relations.

the control volume methodology is based on using simple construction elements to build the total system model, therefore the four component control volumes (including their external interactions) idealize the system.

In choosing the relations that will be sufficient to describe the system being idealized, careful thought must be employed. If an engineering system is not completely specified in terms of the relevant behavioral relations, then the number of additional arbitrary parameters that must be specified will equal the number of degrees of uncertainty left in the mathematical representation of the physical system. On the other hand, if the system is overspecified, ambiguous and contradictory results will precipitate (i.e. over-constrained, physical incompatibility). There must be a compatibility between the physical and mathematical problem: the number of independent unknowns must equal the number of independent relations. One of the obstacles of this effort was in finding this delicate balance between the mathematical and physical requirements.

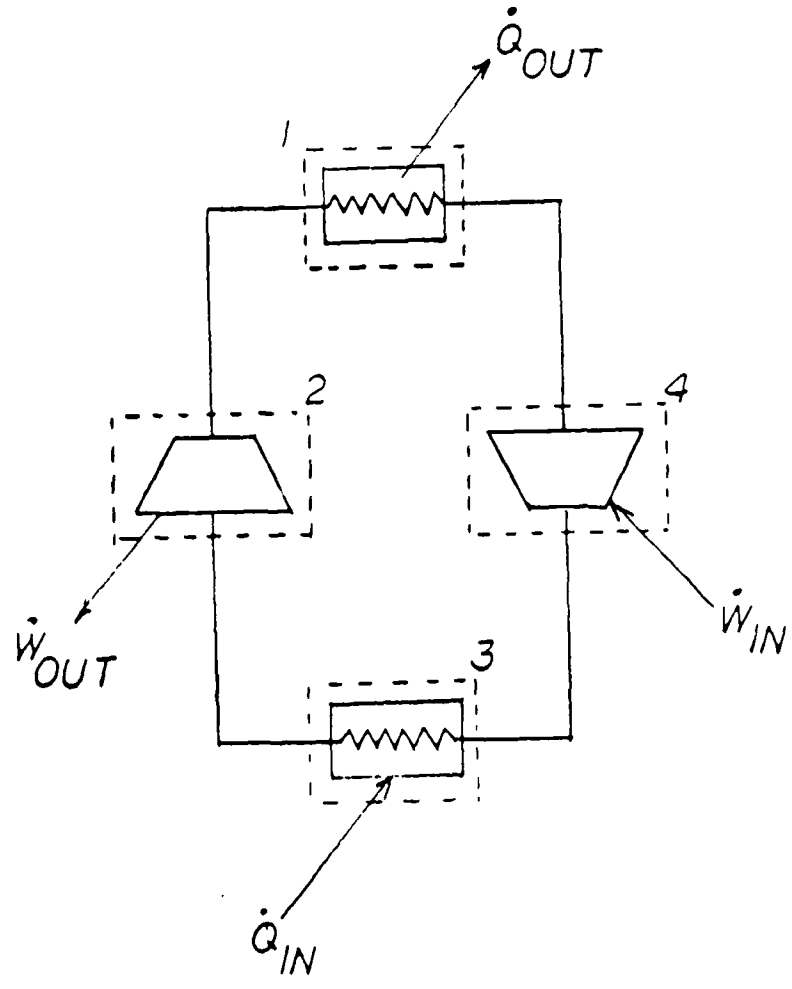

Figure 1. : Conventional representation for analysis of a thermal circuit

2.3.1 Local and Global Variables

Local variables are independently defined within each storage element and are used in the constitutive relations of each storage element. When elements are assembled together to form a system, the local variables are now transformed into a variable system defined for the complete physical system. This system of variables is called the *global* variables system and it is defined only for a specific system based on the specific interconnections between storage elements.

2.3.2 Storage Elements

A storage element is in a pragmatic sense a self-contained standard engineering component such as a turbine, heat exchanger or valve that is defined on an elemental basis. Storage elements transfer energy, entropy, and mass to achieve some desired engineering effect. Accordingly, the 1st Law of Thermodynamics, continuity requirements, and an efficiency (irreversibility parameter) relation are chosen to describe the constitutive behavior of the element.

For devices which exchange work with their environment, the classical definitions of component isentropic efficiency serves as the irreversibilty parameter. Such a definition reflects 2nd Law irreversibilities while incorporating component specific "test-stand" data.

The irreversibility relation for devices which exchange heat (either internally or with the environment) is from the heat transfer rate equation. The irreversibility information is contained in the overall heat transfer coefficient (U) and the available heat transfer area (A) which are used in the rate equation to relate fluid stream

temperatures. A second irreversibility parameter is from the fluid friction losses. Thus, relations defining the pressure drop through a heat exchanger together with the heat transfer rate equation define the irreversibility (entropy generation). This model may seem to make the methodology more complex, but it achieves the goal of incorporating hardware performance data into the elemental models.

The equations used to specify the irreversibilties are called the characteristic relations since they reflect component's characteristic behavior.

The working fluid constitutes an additional constitutive relation for each fluid state. The type of working fluid employed should be arbitrary in a useful analysis method. The physical properties of the fluid should be expressible as a function of independent variables. This has been accomplished for the actual fluid states, but for the isentropic outlet states (work transfer devices), working fluid properties are expressed as a function of the independent pressure variable and the value of the isentrope. That is, $h_{out}=h(P_{out}, s_{in})$.

If a system uses a single working fluid, then all states are calculated using the same property relation. On the other hand, if circuit contains multiple, independent fluid loops each employing different fluids(e.g. a nitrogen pre-cooler for a liquid helium plant), then a fluid designation must be associated with each loop. In other words, each fluid loop would have a working fluid constitutive relation applicable to that fluid. This is more efficient than defining the fluid constitutive behavior for every element.

In summary, each storage element has constitutive relations grouped categorically by 1st Law, characteristic relations, mass continuity and working fluid constitutive behavior.

2.3.3 Interconnective Elements

The interconnective elements model (through their constitutive relations) the linking of various storage elements which constitute the system. As individual components are assembled with their associated elemental constitut ve relations and local variables, a transformation is necessary to shift from the local variables system to the global variables system. Such a transformation is accomplished by the interconnective element's constitutive relations. By transforming from a local to a global variables system, topological information is implicitly contained in the new variables system. The interconnectivity requirements (i. e. the constitutive relations of the interconnections) enforce on the system the equality of independent local variables at a nodal connection between storage elements. Since these local variables are equal, they assume the global variable label at the node. This ensures component interaction. For example, in Figure 1, the outlet pressure from the compressor must equal the inlet pressure to the high temperature heat exchanger. The two local variables are equal and are assigned the global pressure variable. Similar operations are performed on all the independent variables (Chapter 3). When the transformation is complete, the number of global variables equals the number of local variables less the number of interconnection constitutive relations.

2.4 Equation Generation

The constitutive relations of the system are expressed as the $\{R(x_i)\}$ vector which is derived from the constitutive relations of the elements and the topology of the system.

Equation generation refers in this context to the generation of the $[K^t(x_i)]$ matrix and the $\{R(x_i)\}$ vector. These quantities are generated through recursive relations which draw on topological information to generate the appropriate elements of both $[K^t(x)]$ and $\{R(x)\}$. The methods for generating these relations are discussed in further detail in Chapter 6.

2.5 Solution

The solution technique, briefed in Section 2.1 is a Newton's method tailored for this application and will be reviewed in further detail in Chapter 7.

3 Variables and Parameters Management

3.1 Selection of Independent Variables

Section 2.2 made indirect reference to the properties of temperature and pressure as the independent thermodynamic variables of this method. In fact, a significant portion of the CV algorithm development was performed with temperature and pressure as the independent variables. However, temperature and pressure are intensive thermodynamic properties. Two intensive properties can fix the thermodynamic state in a homogeneous, single phase system only. In generalizing this algorithm to an operating refrigeration cycle, determination of properties and states in a binary or two phase system is necessary, since much of the refrigeration effect results from the latent heat. Therefore, to lend generality to the algorithm, pressure and specific volume were selected as two independent variables.

For shaft work machinery(turbines, compressors, etc), three equilibrium states are of interest. The equilibrium inlet state, the isentropic outlet state and the actual outlet state. The isentropic outlet state can be determined as a function of the inlet entropy value and outlet pressure value: $h_{2s}=h(P_2,s_1)$, where $s_1=s_1(P_1,v_1)$.

In addition to pressure and specific volume, mass flow rate has also been selected as an independent variable. Mass flux scales the system's energy and entropy interactions. Mass flow rate is an essential variable when devices such as splitting valves and mixing/recombination valves are employed.

These three variables (pressure, specific volume, mass flow rate) taken together with the interconnectivity relations (between devices) ensure full thermodynamic matching at the "nodes" between storage elements. Thus, a complete engineering link is made between two devices exchanging fluid energy.

3.2 Dependent Variables

The dependent state variables are all other thermodynamic properties:

$h(P,v)$

$h_s(P,s(P,v))$

$s(P,v)$

$T(P,v)$

Work and heat transfer are also system unknowns, although not variables perse. They are determined by the equilibrium values of the global variables. The 1st Law residual functions and $[K^t]$ entries for elements which exchange heat or work with the environment are not incorporated as part of equation (1) framework. Such relations are assigned to a post-processing routine. In doing this, no specificity of the $[K^t(x)]\{\Delta x\}=\{R(x)\}$ equilibrium equation is lost since elimination of a 1st Law relation also eliminates either a work transfer or heat transfer unknown.

Determination of the equilibrium state variables $\{x\}$ completely defines the state of the system, from which heat and work interactions can be determined.

3.3 System Parameters

System parameters are user defined as part of the algorithm initialization where the specifications of component data are imported for use in the applicable constitutive relations. Such parameters include component efficiencies (η_t,η_c), friction factors (f), heat transfer coefficients (U), heat transfer areas (A), and expansion/compression ratios (r_E, r_c).

4 Device Models for Control Volume Analysis

4.1 General

A set of constitutive relations for the individual control volumes has been developed which fit into a standardized framework based on the engineering principles discussed in Chapter 2. The constitutive relations are grouped categorically into 1st Law, continuity, interconnectivity and characteristic relationships (characteristic relations describe the non-ideal behavior of the selected control volume in view of the Second Law irreversibilities that degrade the system performance from the ideal case). The categorical standardization of the relations for different types of engineering devices is necessary to facilitate the assembly of the elements of $[K^t(\{x\})]\{\Delta x\}=\{R(\{x\})\}$ via numerical methods.

4.2 Engineering Devices

The following devices have been selected for implementation in the control volume analysis:

Regenerative Heat Exchangers

Ambient Heat Exchangers

Compressors

Expanders

Expansion Valves

While this list is not all-inclusive, it is representative of typical devices found in cryogenic refrigeration systems and thermal power systems in general. More complicated devices such as stirling engines are not covered here but may be included upon extension of the constitutive framework discussed in Chapter 2.

4.3 Component Constitutive Relations

Symbology for the expander is shown in Figure 2.

1st Law: $$\dot{m}_1 h_1(P_1, v_1) - \dot{m}_2 h_2(P_2, v_2) = \dot{W}_E$$

Characteristic relations:

$$(h_1 - h_2) - \eta_i(h_{1s} - h_{2s}) = 0$$

$$h_1 - h_{1s} = 0$$

$$s_{2s} - s_1 = 0$$

The first equation is the definition for isentropic efficiency. The second equation is a consequence of the recursion used to generate the efficiency equation: h2s can not be numerically generated without generating h1s. This is because the recursive relations use topological information to generate the appropriate functions. Topological information can discriminate between inlet and outlet states but not between isentropic and actual states. The recursion generates an isentropic inlet state which is identical to the actual inlet state; the second equation merely sets the two states equal. The third equation equates the inlet entropy to the outlet entropy for an isentropic process(which must be known to use the efficiency definition). S_{2s} is used in a fluid constitutive relation to determine $h_{2s}=h(P_2, s_{2s})$.

continuity: $$\dot{m}_1 - \dot{m}_2 = 0$$

working fluid: $$h_{2s} - h(P_2, s_{2s}) = 0$$

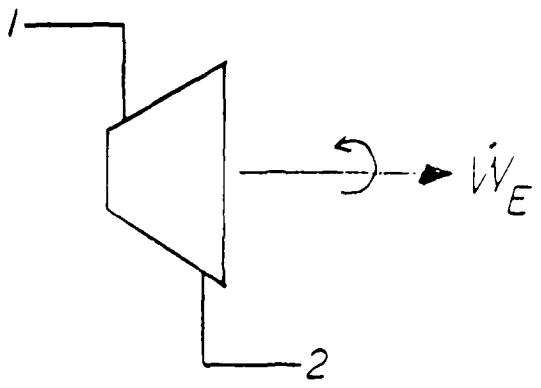

Fig 2. : Expansion Engine Schematic

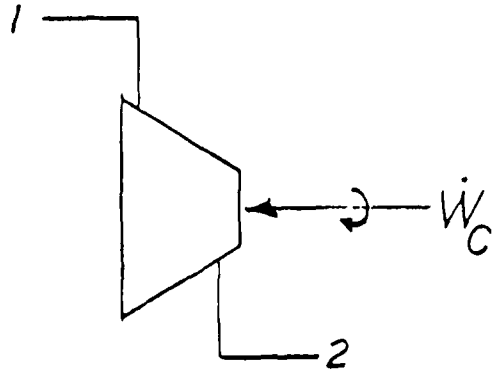

Fig 3. : Compression Engine Schematic

The working fluid constitutive relation defines the outlet enthalpy for the isentropic process.

The nine unknowns in these equations (two mass fluxes, two pressures, two specific volumes, an isentropic enthalpy and entropy and work rate) are represented by only six equations. Since each control volume is a basic building element of the CV algorithm, each individual control volume should be algebraically independent. Therefore three additional equations are necessary - these equations come from the interconnectivity requirements for pressure, specific volume and mass rate. Each (2-port) control volume will have associated with it three interconnectivity relations (from an adjacent interconnective element) which add to the other constitutive relations to ensure algebraic uniqueness.

The applicable constitutive relations can also be developed for the compressor engine, which is schematically shown in Figure 3.

1st Law:

$$\dot{m}_1 h_1(P_1, v_1) - \dot{m}_2 h_2(P_2, v_2) = \dot{W}_C$$

Characteristic relations:

thermal characteristic:

$$\eta_c(h_1 - h_2) - (h_{1s} - h_{2s}) = 0$$

$$h_1 - h_{1s} = 0$$

$$s_{2s} - s_1 = 0$$

pressure characteristic: $$P_1 - r_C P_2 = 0$$

mass continuity:

$$\dot{m}_1 - \dot{m}_2 = 0$$

working fluid:

$$h_{2s} - h(P_2, s_{2s}) = 0$$

These equations are similar to those for the expander, accept that a pressure rise relation (which sets the system pressure levels) has been incorporated.

A schematic for the regenerative heat exchanger is shown in Figure 4.

1st Law:

$$\dot{m}_1 h_1(P_1, v_1) - \dot{m}_2 h_2(P_2, v_2) + \dot{m}_3 h_2(p_3, v_s) - \dot{m}_4 h_4(p_4, v_4) = 0$$

thermal characteristic:

$$\dot{m}_1 h_1 - \dot{m}_2 h_2 - \mathrm{U_R A_R} \ln\left\{\frac{(T_1 - T_4) - (T_2 - T_3)}{(T_1 - T_4)/(T_2 - T_3)}\right\} = 0$$

pressure characteristic:

$$P_1 - P_2 - \left(\frac{16fl}{\pi D^3}\right)_{12} \dot{m}_1^2 (v_1 + v_2) = 0$$

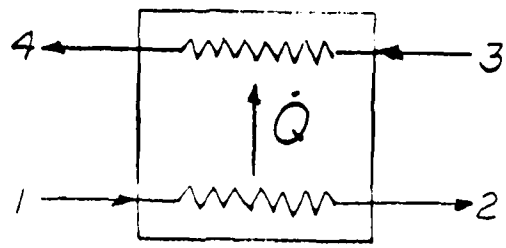

Fig 4. : Regenerative Heat Exchanger Schematic

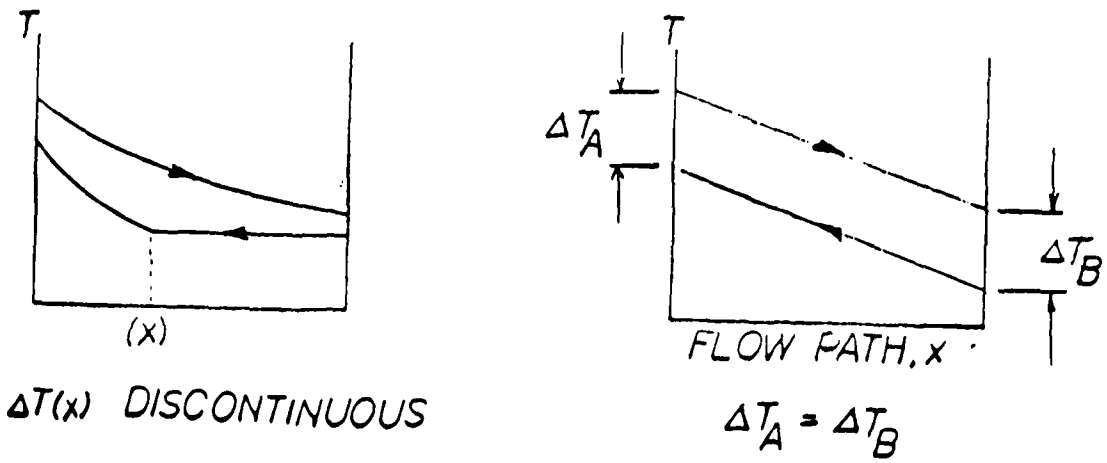

Fig 5. : Temperature profiles for which the rate equation is invalid

$$P_3 - P_4 - \left(\frac{16fl}{\pi D^3}\right)_{34} \dot{m}_3^2 (v_3 + v_4) = 0$$

continuity:

$$\dot{m}_1 - \dot{m}_2 = 0 \qquad\qquad \dot{m}_3 - \dot{m}_4 = 0$$

The temperature characteristic is a form of the rate equation. Stream 1-2 is assumed to be the warm stream and stream 3-4 is the cold stream. It is a valid representation of the temperature profile through a heat exchanger for profiles that exhibit a continuous, exponential temperature difference along the flow path. Figure 5 shows temperature profiles for which the rate equation is not valid: discontinuity in the profile or invariant profile. In instances where a phase change occurs, two separate rate equations should be used, one for each side of the discontinuity. For an invariant profile, the rate equation is valid by taking a limit when ΔTa/ΔTb goes to 0/0. "UA" is the component heat transfer coefficient and heat transfer area.

Two pressure relations are given here for the friction loss phenomena. For model development, the pressure drop is simply represented by a flow duct with characteristic hydraulic diameter, flow path and friction loss factor, which should be known apriori for a given component. This is a very generic representation of pressure drop due to friction.

The segregation of the characteristic equations for this device into temperature and pressure relations does not imply the independence of heat and momentum transfer. On the contrary, they are intimately coupled, which would be reflected by their respective values for "f" and "UA".

An ambient heat exchanger is shown schematically in Figure 6. The constitutive relations for an ambient heat exchanger are very similar to those for the regenerative heat exchanger with the second flow stream being replaced by a quantity of heat being rejected to/ received from the environment.

1st Law:

$$\dot{m}_1 h_1(P_1, v_1) - \dot{m}_2 h_2(P_2, v_2) = \dot{Q}$$

temperature characteristic:

$$\dot{m}_1 h_1 - \dot{m}_2 h_2 - \mathrm{U_A A_A} \ln\left\{\frac{(T_\infty - T_2) - (T_\infty - T_1)}{(T_\infty - T_2)/(T_\infty - T_1)}\right\} = 0$$

pressure characteristic:

$$P_1 - P_2 - \left(\frac{16fl}{\pi D^3}\right)_{12} \dot{m}_1^2 (v_1 + v_2) = 0$$

continuity:

$$\dot{m}_1 - \dot{m}_2 = 0$$

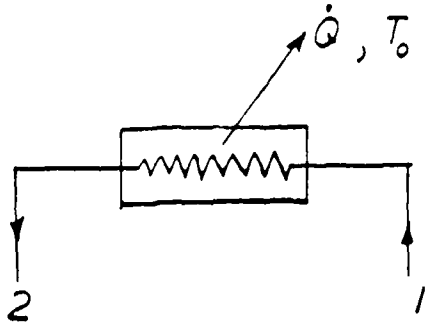

Figure 6. : Ambient Heat Exchanger Schematic

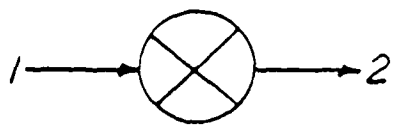

Figure 7. : Expansion (Throttling) Valve

The relations for the ambient heat exchanger are of the same form as those for the regenerative heat exchanger. A subtle difference exists in that the ambient environment is represented by a temperature reservoir T_∞. At steady state or for very large reservoirs (i.e. $m_{reservoir} >> m_{sys,tot}$), T_∞ is invariant. T_∞, f and $U_A A_A$ are also defined during initialization.

The last device which is commonly found in cryogenic systems is the throttling or expander valve, shown schematically in Figure 7.

1st Law:

$$\dot{m}_1 h_1(P_1, v_1) - \dot{m}_2 h_2(P_2, v_2) = 0$$

characteristic relation:

$$h_1 - h_2 = 0$$

continuity:

$$\dot{m}_1 - \dot{m}_2 = 0$$

The principle characteristic of the expansion valve is that the entering and exiting enthalpies are equal (although the enthalpy through the valve is not constant). Note that the pressure drop across the valve is not specified as a characteristic relation. In order for the existence of this valve to make physical sense in a refrigeration system, it must operate in conjunction with a pressure elevating device (compressor). Placing a required pressure

ratio on the expansion valve would place a redundant overconstraint on the system, since the compressor already sets the system's principal operating pressure levels (see Section 2.2:Compatibility).

4.4 Interconnectivity Relations

The interconnectivity relations are mathematically trivial but form the critical link to the algorithm. By equilibrating the independent thermodynamic variables between the outlet of one device and the inlet of a connected device, thermodynamic matching is imposed on the system. Now, all elements behave in a highly-coupled interactive manner.

Interconnectivity places three relations at each component interface: pressure, specific volume and mass flux. Equilibration of pressure and specific volume ensure a thermodynamic match of the working fluid and equilibration of mass flux closes the continuity loop around a closed system. Typically, interconnectivity relations will have form

$$P_2 - P_3 = 0 \qquad v_2 - v_3 \qquad \dot{m}_2 - \dot{m}_3 = 0$$

4.5 Summary

The device models presented here are self-contained, problem-independent equation sets. The next task is to shape the constitutive relations so that they may be compatible for assembly of the [K'] matrix and the {R} vector.

5 Topology

5.1 Introduction

Prior to discussing the assembly of the [K^t] matrix and {R} vector, it is useful to describe how the topology is developed, since [K^t] and {R} are assembled using the system's topolgy. The topology establishes in mathematical terms which elements are connected and how they are connected in an engineering system. Different types of interactions yield different topological structures or networks.

The most efficient numerical method of representing the system topology is with the topology or incidence matrix. Such a matrix is a tertiary state (1, 0 or -1) matrix that relates the connectivity of nodal variables. Topology matrices are commonly found in discrete network systems such as electrical network circuits exchanging current or structural networks exchanging displacements. In the Control Volume methodology, topology is used to describe how elements exchange mass, energy and entropy. Hence, there is more than one interaction at each node. Figure 8 shows a typical structural network. The springs represent elements that store energy; the nodes represent equipotential points between storage elements. The topology matrix for this system is

$$Top[i,j] = \begin{bmatrix} 1 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -1 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix}$$

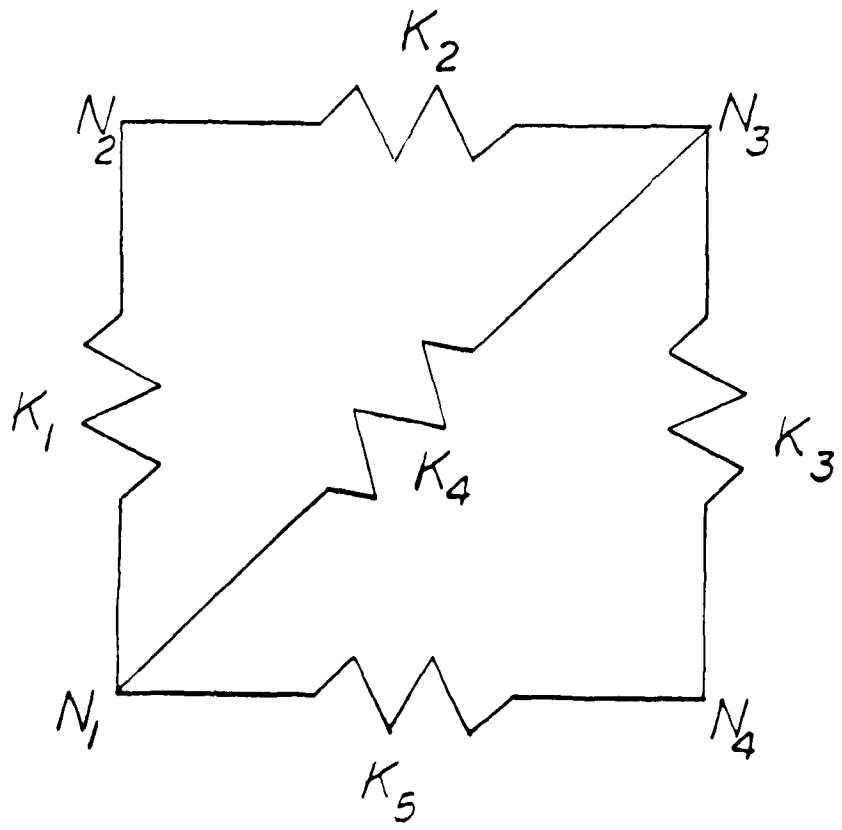

Figure 8. : A structural network; k_i represent elemental stiffnesses

The columns represent nodes (interconnective elements) and the rows represent storage elements. In the CV algorithm, topology is defined on two levels: thermal and mass exchange. Thermal topology describes elements in thermodynamic communication: storage elements exchanging heat, work, fluid energy and entropy. The mass exchange topology describes the arrangement of elements exchanging mass and momentum.

Why is this done? It is principally a matter of mathematical convenience for the assembly of the appropriate residual functions and $[K^t]$ functions. The thermal topology is used to assemble the 1st Law and temperature characteristics, while the mass topology matrix is used to assemble the pressure characteristic and mass continuity relations. The distinction arises due to the presence of counterflow heat exchangers that have one 1st Law relationship and one temperature characteristic but two pressure loss functions and two mass flow relations. In such an arrangement, the two separate flow passages in a counterflow heat exchanger each constitute a separate pressure loss mechanism. But only one energy interaction is present.

The computer will generate these matrices by scanning screen. However, the initialization routine will require two separate topological generations, one on the thermal interaction level and one on the mass transfer interaction level.

As an example of the application of the control volume toplogy, consider the Claude cycle shown in Figure 9. Five storage elements and six interconnective elements (nodes) are shown. This system will have five 1st Law relations and thermal interaction characteristics, but six momentum interactions since there are six distinct flow passages. The thermal topology matrix is

$$[Top_T] = \begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & -1 \\ 1 & -1 & 0 & 1 & -1 & 0 \\ 0 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \end{bmatrix}$$

The mass and momentum exchange topology matrix is given here for the same Claude cycle, but the schematic difference is shown in Figure 10. The distinct flow circuits of the regenerative heat exchanger are now modelled as separate entities such that the corresponding topology can be used to generate the pressure characteristic relations and the mass flux relations.

$$[Top_m] = \begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 1 & -1 & 0 \\ 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \end{bmatrix}$$

The convention used in both topological representations is taken as flow into an element as positive and flow out of an element as negative.

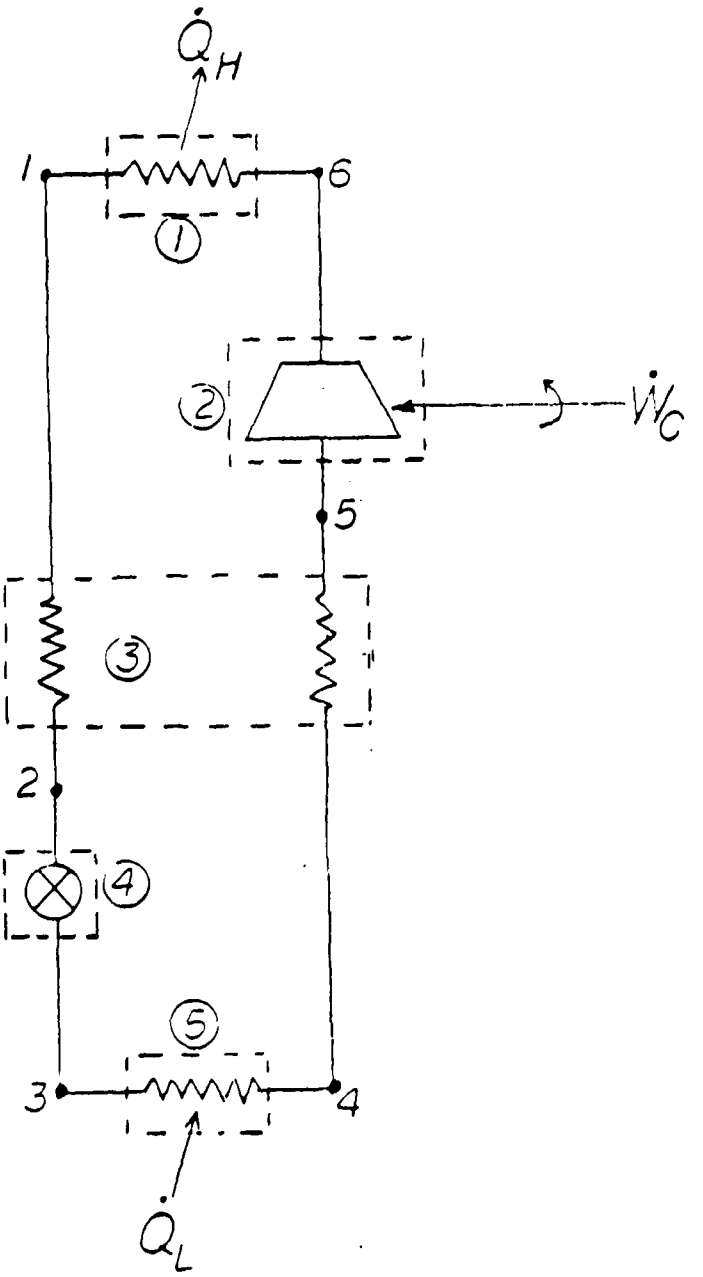

Figure 9. : Thermal topology representation for a Claude cycle:

six nodes, 5 storage elements.

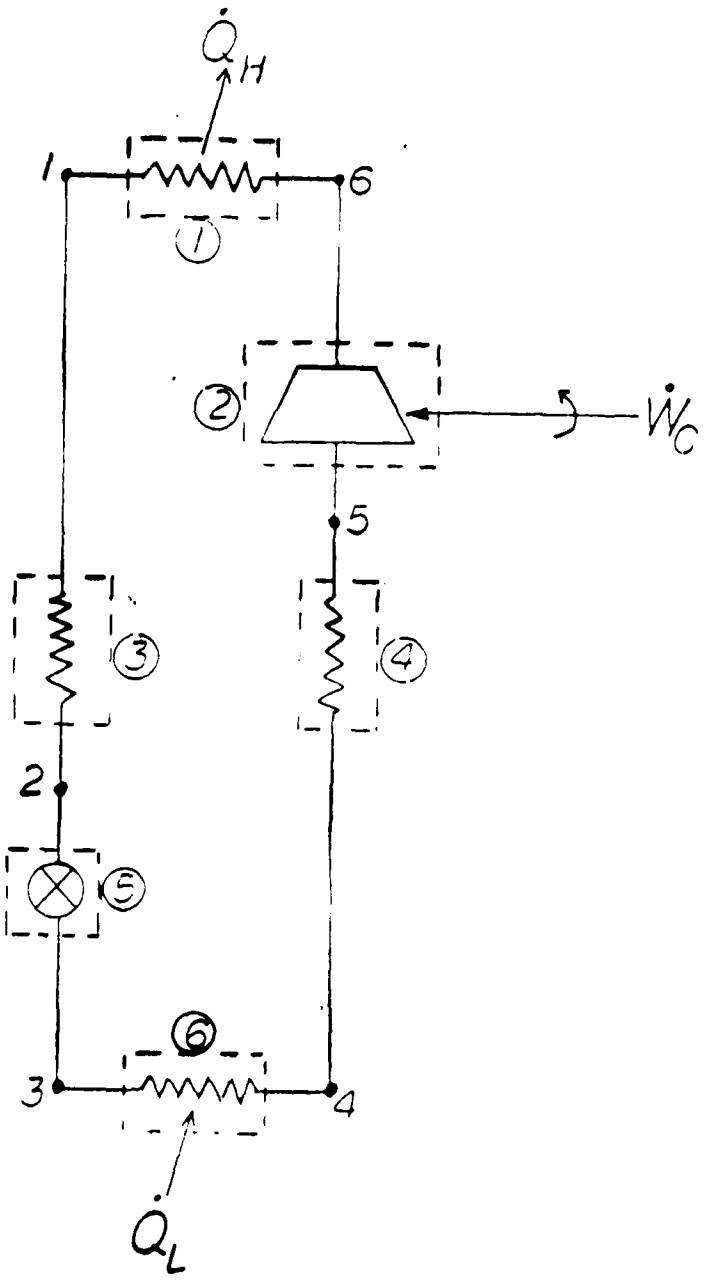

Figure 10. : Mass topology representation for a Claude cycle:

six nodes, six storage elements.

6 Generation of the Residual Relations

6.1 Introduction

Chapter's 4 (elemental models) and 5 (topology) laid the mathematical foundation for the constitutive relations that serve as the basis for generating the $[K^t]$ matrix and the $\{R\}$ vector. The algebraic equation sets presented in Chapter 4 must be manipulated to conform to the numerical requirements of $[K^t(x_i)]\{\Delta x\}=\{R(x_i)\}$. The $[K^t]$ matrix is generated from the elemental constitutive relations in two steps. Since $[K^t]$ is a Jacobian of the system residual relations, the first derivatives (with respect to the global variables) of all the elemental constitutive relations must be computed and these first derivatives are the constitutive relations of the elements assigned to their proper $[K^t]$ locations. This is done using the system topology information.

6.2 Assembly of the {R(x)} Vector

$\{R\}$ is the array used to determine the steady state operating conditions of the system. It is also assembled using the system topology information.

The assembly of the $\{R\}$ vector is much simpler than the assembly of the $[K^t]$ matrix (Section 6.4). A subtle differences between the generation of $\{R\}$ and $[K^t]$ is that the residual relations $\{R(x)\}$ are multiple function equations(e.g. a 1st Law has several $\dot{m}_i h_i$ arguments summed together). Hence, their recursive relations shall contain summation operators to cycle through the nodal variables and use the topology to filter out entries that are not pertinent to the specific residual. On the other hand, the elements in the [Kt] matrix are usually single-argument entities (e.g.$\frac{\partial h_1}{\partial P_2}$)-no summation over the range of nodal variables is made.

As an example, consider the 1st Law relation for the regenerative heat exchanger shown in Fig. 10:

$$\dot{m}_1 h_1 - \dot{m}_2 h_2 + \dot{m}_4 h_4 - \dot{m}_5 h_5 = R$$

The thermal topology array (row) for the element in question will contain (+1) for the flows (from nodes) entering the element, (-1) for flows (to nodes) exiting elements and (0) for nodes not connected to the element under consideration. The regenerator in Fig. 10 corresponds to storage element 3, which corresponds to row 3 in the thermal topology matrix $Top_T[3,j]$ shown on page 42. Thus,

$$Top_T[3,j] = [1 \quad -1 \quad 0 \quad 1 \quad -1 \quad 0]$$

$$R = \sum_{j=1}^{6} \dot{m}_j h_j Top_T[3,j]$$

where 6 equals the number of nodes in the system. Expanding the summation through the appropriate values of 'j' (and hence $Top_T[3,j]$) yields

$$\dot{m}_1 h_1 - \dot{m}_2 h_2 + \dot{m}_4 h_4 - \dot{m}_5 h_5 = R$$

Similar combinatorial operations can be performed to generate all the residual functions. However, not all constitutive relations have such well regimented structures as the additive 1st Law. In such cases, the numerical value of the topological arguments are used to modify the variable indexes and parameters where appropriate. This is apparent in the pressure characteristic constitutive relation (Section 4.3) where one pressure is multiplied by the pressure ratio and the other pressure is not.

$$P_1 - r_c P_2 = 0$$

The topolgy value (1 or -1) can be used to ensure that the pressure ratio multiplier appears only with the outlet pressure. The details of the recursion relations used to develop the {R} vector are left o Appendix 1.

6.3 [K^t] Matrix Functions

The analytical functions that form the entries in [K^t] matrix are the first derivatives (with respect to the global independent variables) of the residual functions:

$$K_{ij}^t = \frac{\partial R_i}{\partial x_j}$$

Taken literally, the residual functions R_i must be known prior to computing K^t_{ij}. This would be the case for analytical generation of [K^t], but the control volume method is numerically based for implementation on a computer. It would not be the best employment of a computer's potential to generate and store all the system's residual relations and then compute their derivatives. It would be prudent to store the unspecified first derivative constitutive relations (which are standardized for each element type) and then form system specific constitutive relations from these standardized relations by combination with the system topologies. This is precisely the what is done here.

As discussed in Chapter 4, all the possible "R's" are limited to 1st Law, thermal and pressure characteristics and mass continuity relations for a limited collection of elements (Sect. 4.1). x_i are the system global parameters, namely pressure, specific volume, mass and flow rate at each interconnection. As an example, a 1st Law relation for a regenerative heat exchanger is developed as follows:

$$R_i(x_j) = \sum_{j=1}^{p} \dot{m}_j h_j = 0$$

where p represents the number of fluid streams entering or leaving the control volume for device "i". The partials of R with respect to one set of system global parameters are:

$$\frac{\partial R_i}{\partial P_j}, \qquad \frac{\partial R_i}{\partial v_j}, \qquad \frac{\partial R_i}{\partial \dot{m}_j}$$

These derivative functions have the following standard form:

$$\frac{\partial R_i}{\partial P_j} = \sum_{j=1}^{p} \dot{m}_j \frac{\partial h_j}{\partial P_j}]_v$$

$$\frac{\partial R_i}{\partial v_j} = \sum_{j=1}^{p} \dot{m}_j \frac{\partial h_j}{\partial v_j}]_p$$

$$\frac{\partial R_i}{\partial \dot{m}_j} = \sum_{j=1}^{p} h_j$$

where the right hand side of the equations contain only constitutive relations and global variables. The use of the topology matrices for the generation of the [K^t] terms is presented in Appendix 1.

As mentioned in Section 2.3.2, 1st Law relations with heat and work transfer are not incorporated into the K^t framework, so no derivatives need be computed for $\dot{W}$ or $\dot{Q}$ terms. $\dot{W}$ And $\dot{Q}$ computation is assigned to post-processing.

Finally a numerical (instead of an analytical) derivative is used to represent the linearization of the rate equation (heat exchanger).

6.4 Assembly of the [K^t] Matrix

6.4.1 Interaction Regions of the [K^t] Matrix

The constitutive relations that form the [K^t] matrix described in Section 6.3 are the basis for the formulation of the [K^t] terms.

To develop [K^t], it is necessary to visualize the matrix consisting of separate interaction regions each corresponding to a type of interaction as described in Section 2.3.2 and Chapter 4: 1st Law, thermal characteristics, pressure characteristics, and mass continuity.

$$[K^t(x)]\,\{x\} = \begin{bmatrix} \text{1st Law} \\ \text{temp. characteristic} \\ \text{Pres. characteristic} \\ \text{mass continuity} \end{bmatrix} \{x\}$$

This administrative subdivision of the [K^t] matrix is necessary due to the two differing types of interaction that lead to two distinct topology matrices: thermal and mass exchange. The vector {x} is the collection of the independent variables relevant to the problem: $\{P_1, P_2, \ldots, P_n, v_1, v_2, \ldots, v_n, \dot{m}_1, \dot{m}_2, \ldots, \dot{m}_n\}$. The derivative functions presented in Appendix 1 must now be uniquely assigned to their appropriate location in [K^t] using the topological information.

Since there will only be three types of independent variables, each interaction region within the [K^t] matrix may be further subdivided (in an administrative sense) into smaller 2nd-order arrays.

$$
[K'(x)]\,\{x\} =
\begin{array}{l}
(R_i = \text{1st Law}) \\
(R_i = \text{therm. char.}) \\
(R_i = \text{pres. char.}) \\
(R_i = \text{mass cont.})
\end{array}
\begin{bmatrix}
\left[\frac{\partial R_i}{\partial P_j}\right] & \left[\frac{\partial R_i}{\partial v_j}\right] & \left[\frac{\partial R_i}{\partial \dot{m}_j}\right] \\
\left[\frac{\partial R_i}{\partial P_j}\right] & \left[\frac{\partial R_i}{\partial v_j}\right] & \left[\frac{\partial R_i}{\partial \dot{m}_j}\right] \\
\left[\frac{\partial R_i}{\partial P_j}\right] & \left[\frac{\partial R_i}{\partial v_j}\right] & \left[\frac{\partial R_i}{\partial \dot{m}_j}\right] \\
\left[\frac{\partial R_i}{\partial P_j}\right] & \left[\frac{\partial R_i}{\partial v_j}\right] & \left[\frac{\partial R_i}{\partial \dot{m}_j}\right]
\end{bmatrix}
\begin{Bmatrix}
P_1 \\ P_2 \\ \cdot \\ \cdot \\ P_n \\ v_1 \\ v_2 \\ \cdot \\ \cdot \\ v_n \\ \dot{m}_1 \\ \dot{m}_2 \\ \cdot \\ \cdot \\ \dot{m}_n
\end{Bmatrix}
$$

Each array denoted by [ ] represents the collection of 1st derivatives of a constitutive relation with respect to one of the independent variables. The six arrays corresponding to 1st Law and thermal characteristic are identical in size to the thermal topology matrix, used to assemble the arrays from the constitutive relations of the elements. Similarly, the six arrays corresponding to pressure characteristic and mass continuity use the mass topolgy matrix for function generation. All arrays have the same number of columns (since each column represents a node), which ensures the columns properly align when the total [K^t] matrix is assembled.

The justification for this arrangement within the [K^t] matrix is that it makes assembly of the matrix simpler. Once the respective toplogy matrices are established,

each storage element is queried for its applicable constitutive relations (which form {R}) and [K^t]. These relations are combined with the topology through recursive relations to define, in this case, the appropriate [K^t] entry.

6.4.2 Array Assignments

Each array shall be labelled using the following convention for ease in identifying what interactions it represents, where it should be assigned in [K^t], and for establishing the recursions used to produce the [K^t] entires. The first superscript "t" indicates (as before) that the functions to be developed consist of terms of the system tangent stiffness matrix. The second superscript indicates the interaction type to which this array refers(1st Law =1, therm. char.=T, pres. char=P, mass cont.=m. The first subscripts are the array location indices. The outer subscript indicates the respective variable of derivation (P, v or $\dot{m}$). As an example, consider

$$(K^t_{34})^1_p$$

Superscript "1" means that this array refers to a 1st Law relation. Subscript "P" indicates that the functions inside are the partial derivatives with respect to the independent pressure variable. The indices [3,4] indicate that this particular entry corresponds to the third 1st Law relation and the fourth global pressure. This labelling has been developed so that each inner matrix can be developed independent of the next one using the recursive relations that are to be presented in the following paragraphs. Using this identification scheme, The [K^t] matrix has as arrays

$$[K^t] = \begin{bmatrix} [K_{ij}^t]_p^1 & [K_{ij}^t]_v^1 & [K_{ij}^t]_{\dot{m}}^1 \\ [K_{ij}^t]_p^T & [K_{ij}^t]_v^T & [K_{ij}^t]_{\dot{m}}^T \\ [K_{ij}^t]_p^P & [K_{ij}^t]_v^P & [K_{ij}^t]_{\dot{m}}^P \\ [K_{ij}^t]_p^m & [K_{ij}^t]_v^m & [K_{ij}^t]_{\dot{m}}^m \end{bmatrix}$$

The partial derivative functions of the constitutive relations of Appendix 1 (discussed in Section 6,3) are combined with the respective topology matrices to form the inner matrices, which form the global [K^t] matrix. Each row within an inner matrix corresponds to the derivative of a storage element's constitutive relations.

As an example, the recursive relations to generate the inner matrices for the 1st law interactions are:

$$(K_{ij}^t)_p^1 = \dot{m}_j \frac{\partial h_j}{\partial P_j}]_{v_j} \mathrm{Top}_T[i,j]$$

$$(K_{ij}^t)_v^1 = \dot{m}_j \frac{\partial h_j}{\partial v_j}]_{P_j} \mathrm{Top}_T[i,j]$$

$$(K_{ij}^t)_{\dot{m}}^1 = h_j \mathrm{Top}_T[i,j]$$

The recursive relations for all inner matrices are contained in Appendix 3.

6.4.3 Summary

The [K^t] matrix has been subdivided for assembly purposes into interaction regions and inner arrays corresponding to the global variable. Each inner array is generated by a recursion relation (App. 2) standardized for each type of control volume.

Any inner matrix may be identically zero if the constitutive relations (for that array) are not functions of the variable used to compute the partial derivatives. Each $[K^l]$ term is a function of constitutive relations of the elements.

Thermal toplogy is used to generate 1st Law and thermal characteristic functions while the Mass topology is used to generate the pressure characteristic and mass continuity functions. If a system is composed entirely of two-port elements, then the mass and thermal topology matrices will be identical. In the general case however, the index ranges for the two matrices will be different.

7 Chronology of CV Method

7.1 Introduction

The formulation and solution procedure has three steps: preprocessing, generation (system assembly) and reduction.

7.2 Preprocessing

The first step in the preprocessing operation is to establish the control volumes of interest in a closed loop system. During the initialization of each individual storage element local variables are assigned based on the type of element, i.e. a standard two-port element (expander) will have inlet variables P^1 , v^1 , $\dot{m}^1$ and outlet variables P^2 , v^2 , $\dot{m}^2$. A four port element will have $P^1, \ldots, P^4$ etc. The local variable assignment sets the stage for the local to global variable transformation (i.e. system specification) as discussed in Sections 2.3.1, 2.3.3 and 4.4.

These transformations are conducted for all the independent variables (P and v as well) at the interconnecting nodes only. This local to global transform has two functions: (1) it reduces the number of independent state variables by a factor of two thereby making the system algebraically unique and (2) it impresses on the system the interactive requirements of the individual elements.

When the elements that constitute the system are selected and connected per designer's requirements, the interconnectivity is then known and the topology can be established. The topology is then used to generate the applicable matrices and vectors.

7.3 System Assembly

The assembly revolves around the individual control volume as a basic construction element. Once the algorithm determines the number of storage elements and connective nodes (via the topology matrices), it will establish space (memory) sufficient to carry the requisite number of constitutive relations based on the characteristics of each control volume. The details of the assembly operation were discussed in Chapter 6.

7.4 Reduction

Reduction is the actual numerical solution of the $[K^t(x^k)]\{\Delta x^k\}=\{R(x^k)\}=0$ system. It uses a simple Newton-Raphson method to successively iterate toward the equilibrium state, $\{x^{eq}\}$ (the index "k" represents the "kth" numerical value based on thermodynamic state $\{x^k\}$). This method is a common numerical exercise and is discussed in detail in Appendix 4.

8 Conclusions

This effort was the first step in an effort that is to develop new computer-based techniques for the simulation of cryogenic engineering plant performance. This work centered on cycle analysis of steady-flow cryogenic systems. Simulation is the extension of this analysis to more generalized operating scenarios. Analysis is indeed difficult, yet it is only the first step toward simulation. In analysis however, some important foundations can be established (or alternatively, bad foundations can be eliminated) which may be incorporated into simulation models. Such matters concern variable management, idealization of the physical problem, mathematical formulation of the idealization and a solution algorithm. There are some fundamental obstacles which stand in the way of achieving a simulation model for a thermal power system. These obstacles arose during this effort conspicuously and inconspicuously- certain obstacles remain, some were overcome. The remarks that follow address in retrospect the extension of this work to future development and the problems in simulation in general.

Most of the work that has been done in the simulation of thermal power systems has been done in the nuclear power plant field due to the critical need for understanding of plant behavior before embarking on construction. However, most simulation models are limited to a very select set of flow circuits. A methodology to perform analysis (or simulation) of arbitrary thermal circuits has not been rigorously-developed or disseminated. This paper presented a method of analysis for arbitrary thermal power systems.

Another fundamental obstacle in analysis and simulation of power systems lies in the historical practice of thermodynamics. The industrial age has seen the expansion of power sources (electrical, automotive) to all corners of the earth. Accordingly, much of the thermal

power engineering has been design oriented. As a result, thermodynamic models for processes have been tooled to yield design data based on some required performance specification: 1st Law results scale sizes of systems; efficiency definitions dictate what efficiency is required to achieve some net work; rate equations define area and heat transfer requirements for a specified heat transfer. Such models form the cornerstone of time-proven design aids. Design is the antithesis of analysis and simulation, and herein lies the difficulty for the analysis problem: a plethora of good design models, yet a dearth of useful analysis models. What is frequently done is the design models are "reverse-engineered": performance is determined based on specified component design data. The practical application of such an approach has shortcomings.

Design models are basically lumped-parameter relations (whereas steady flow devices usually exhibit gradients. These lumped-parameter models are useful due to their simplicity which was one reason for implementing them in this method: use simple models to build complex systems. More complex elements will be handled in the same way by the processing and solution algorithm. However, as was seen in Chapter 6 (and in the appendices), even these simple models required significant algebraic and numerical manipulation to fit the into framework. Another shortcoming of the lumped-parameter formulation was that it restricted the class of problems to be studied (steady flow systems). To analyze off-design and transient behavior would require models of drastically greater complexity which are not expressible as lumped-parameter elements, whose behavior may or may not be expressible in closed form analytical functions. In effect, the analysis/simulation problem is an enigmatic trade-off between elemental model simplicity and algorithm complexity: a numerically based analysis algorithm begs to be discredited and linear while thermal systems are unquestionably continuous and inevitably non-linear. If element models and their interactive behavior could be

linearized and discredited, then all processes could be simply reduced to differences amongst linear functions of state variables. However, it is well known from the study of thermodynamics that most real processes are path-dependent, rendering such an approach ineffective.

Future study may investigate similar problems in different fields. For example, the finite element analysis of plastic flow and failure of a solid is a problem in continuous, non-linear behavior that has been discredited. However, it differs from the thermal power problem in that a power system may have a various type of constitutive components while a steel truss is constitutively homogeneous throughout its system.

Another approach, as a corollary to the CV method, may be to impose equilibrium at the elements and interpret in some way the mismatch at connecting nodes (the CV approach imposed equilibrium at the nodes and allowed the elements to achieve a local equilibrium). It has been suggested that an initial-value approach be investigated...the number of potential paths is still unknown.

This author wishes to illustrate that this is one approach to the problem, an approach which sought a delicate balance between element simplification and algorithmic complexity. At the expense of sounding reflective, the author feels compelled to share these uncertainties, questions and apprehensions for the edification of future investigators to keep this line of research viable.

Appendix 1 Recursion Relations for Generating the {R} Vector

As in the assembly of [K^t], two topology matrices are used to generate {R}: thermal topology to generate 1st Law and temperature constitutive terms, and mass topology to generate the pressure characteristics and mass continuity.

1st Law:

$$R_i = \sum_{j=1}^{n} \dot{m}_j h_j \mathrm{Top}_T[i,j]$$

The upper summation limit "n" corresponds to the number of nodes in the system.

Thermal characteristic constitutive relation:

For the expander:

$$R_1 = \sum_{j=1}^{n} \{h_j - \eta_t h_{js}\} \mathrm{Top}_T[i,j]$$

$$R_2 = \sum_{j=1}^{n} \{h_j - \eta_t h_{js}\} \mathrm{Top}_T[i,j] \left(\frac{1}{2}\right) \{\mathrm{Top}_T[i,j] + 1\}$$

$$R_3 = \sum_{j=1}^{n} \{s_{(j+\mathrm{Top}_T[i,j])s} - s_j\} \mathrm{Top}_T[i,j] \left(\frac{1}{2}\right) \{\mathrm{Top}_T[i,j] + 1\}$$

For the compressor, the usual substitutions apply.

Pressure characteristic constitutive relation:

For compressors:

$$R_i = \sum_{j=1}^{n} \left[P_j r_E^{-\frac{1}{2}\mathrm{Top}_m[i,j]} \right] \mathrm{Top}_m[i,j] \qquad \text{(expander)}$$

For fluid flow with momentum loss (heat exchangers):

$$R_i = \sum_{j=1}^{n} \left[P_j - \left(\frac{32fl}{\pi D^3} \right) (\dot{m}_j^2) v_j \right] \mathrm{Top}_m[i,j]$$

Continuity constitutive relation:

$$R_i = \sum_{j=1}^{n} \dot{m}_j \mathrm{Top}_m[i,j]$$

Appendix 2 Terms of the [K^t] matrix

The algebraic system described in Chapter 4 must be manipulated to conform to the numerical requirements of the [K^t]{Δx}={R} solution methodology.

Partial derivatives of 1st Law Relations

As mentioned in Section 5.2, 1st law relations that have environmental interactions are not incorporated in K^t. Thus, a first law relation for an adiabatic device with no work transfer can be written

$$R_i(x_j) = \sum_{j=1}^{p} \dot{m}_j h_j = 0$$

where p represents the number of fluid streams entering or leaving the control volume for device "i". P, v and m at each interconnection are the independent global variables. Hence, for each residual relation, the following partial derivatives are of interest:

$$\frac{\partial R_i}{\partial P_j}, \qquad \frac{\partial R_i}{\partial v_j}, \qquad \frac{\partial R_i}{\partial \dot{m}_j}$$

For the 1st Law residual, the previous equations become:

$$\frac{\partial R_i}{\partial P_j} = \sum_{j=1}^{p} \dot{m}_j \frac{\partial h_j}{\partial P_j}$$

$$\frac{\partial R_i}{\partial v_j} = \sum_{j=1}^{p} \dot{m}_j \frac{\partial h_j}{\partial v_j}$$

$$\frac{\partial R_i}{\partial \dot{m}_j} = \sum_{j=1}^{p} h_j$$

These recursive relation will be combined with the topology matrices in Chapter 7 to yield the actual K^t entries.

Partial Derivatives of Characteristic Relations

Expansion engine characteristic functions:

$$(h_1 - h_2) - \eta_t(h_{1s} - h_{2s}) = 0$$

$$h_1 - h_{1s} = 0$$

$$s_{2s} - s_1 = 0$$

Direct differentiation with respect to the independent variables leads to the linearized characteristic functions:

$$\frac{\partial R_1}{\partial P_1} = \frac{\partial h_1}{\partial P_1}\Big]_{v1} - \eta_t \frac{\partial h_{1s}}{\partial P_1}\Big]_{v1} + \eta_t \frac{\partial h_{2s}}{\partial s_{2s}}\Big]_{P2} \frac{\partial s_{2s}}{\partial P_1}\Big]_{v1}$$

$$\frac{\partial R_1}{\partial P_2} = -\frac{\partial h_2}{\partial P_2}\Big]_{v2}$$

$$\frac{\partial R_1}{\partial v_1} = \frac{\partial h_1}{\partial v_1}\Big]_{P1} - \eta_t \frac{\partial h_{1s}}{\partial v_1}\Big]_{P1} + \eta_t \frac{\partial h_{2s}}{\partial s_{2s}}\Big]_{P2} \frac{\partial s_{2s}}{\partial v_1}\Big]_{P1}$$

$$\frac{\partial R_1}{\partial v_2} = -\frac{\partial h_2}{\partial v_2}\Big]_{P2}$$

$$\frac{\partial R_2}{\partial P_1} = \frac{\partial h_1}{\partial P_1}\Big]_{v1} - \frac{\partial h_{1s}}{\partial P_1}\Big]_{v1}$$

$$\frac{\partial R_2}{\partial v_1} = \frac{\partial h_1}{\partial v_1}\Big]_{P_1} - \frac{\partial h_{1s}}{\partial v_1}\Big]_{P_1}$$

$$\frac{\partial R_2}{\partial P_2} = \frac{\partial R_2}{\partial v_2} \equiv 0$$

$$\frac{\partial R_3}{\partial P_1} = \frac{\partial s_{2s}}{\partial P_1}\Big]_{v_1} - \frac{\partial s_1}{\partial P_1}\Big]_{v_1}$$

$$\frac{\partial R_3}{\partial v_1} = \frac{\partial s_{2s}}{\partial v_1}\Big]_{P_1} - \frac{\partial s_1}{\partial v_1}\Big]_{P_1}$$

$$\frac{\partial R_3}{\partial P_2} = \frac{\partial R_3}{\partial v_2} \equiv 0$$

The linearized constitutive relations for the compressor are similar to those for the expander engine and an additional characteristic equation for the pressure elevation term:

$$R_4 = P_1 - r_E P_2 = 0$$

$$\frac{\partial R_4}{\partial P_1} = 1 \qquad \frac{\partial R_4}{\partial P_2} = -r_E$$

Regenerative heat exchanger characteristic equations:

$$R_1 = P_1 - P_2 - \left(\frac{16fl}{\pi D^3}\right)_{12} \dot{m}_1^2 (v_1 + v_2) = 0$$

$$R_2 = P_3 - P_4 - \left(\frac{16fl}{\pi D^3}\right)_{34} \dot{m}_3^2(v_3 + v_4) = 0$$

$$R_3 = \dot{m}_1 h_1 - \dot{m}_2 h_2 - U_R A_R \ln\left\{\frac{(T_1 - T_4) - (T_2 - T_3)}{(T_1 - T_4)/(T_2 - T_3)}\right\}$$

The partial derivatives are:

$$\frac{\partial R_1}{\partial P_1} = -1 \qquad \frac{\partial R_1}{\partial P_2} = 1$$

$$\frac{\partial R_1}{\partial \dot{m}_1} = -\left(\frac{32fl}{\pi D^3}\right)\dot{m}_1(v_1 + v_2)$$

$$\frac{\partial R_1}{\partial v_1} = -\left(\frac{16fl}{\pi D^3}\right)\dot{m}_1^2(1 + v_2)$$

$$\frac{\partial R_1}{\partial v_2} = -\left(\frac{16fl}{\pi D^3}\right)\dot{m}_1^2(v_1 + 1)$$

$$\frac{\partial R_2}{\partial P_4} = -1 \qquad \frac{\partial R_2}{\partial P_3} = 1$$

$$\frac{\partial R_2}{\partial \dot{m}_3} = -\left(\frac{32fl}{\pi D^3}\right)\dot{m}_3(v_3 + v_4)$$

$$\frac{\partial R_2}{\partial v_4} = -\left(\frac{16fl}{\pi D^3}\right)\dot{m}_3^2(1 + v_3)$$

$$\frac{\partial R_2}{\partial v_3} = -\left(\frac{16fl}{\pi D^3}\right)\dot{m}_3^2(1+v_4)$$

Special attention must be paid to the linearization of the rate equation. Obviously,

$$\frac{\partial R_3}{\partial \dot{m}_1} = h_1 \qquad \frac{\partial R_3}{\partial \dot{m}_2} = -h_2$$

Partial derivatives with respect to P and v yield, complex functions that may be replaced by a numerical derivative. To implement this, the chain rule is first applied:

$$R_3 = g(h_i(P,v), T_i(P,v), \dot{m}_i)$$

$$\frac{\partial R_3}{\partial P_i} = \frac{\partial g}{\partial h_i}\frac{\partial h_i}{\partial P_i}]_{v_i} + \frac{\partial g}{\partial T_i}\frac{\partial T_i}{\partial P_i}]_{v_i}$$

$$\frac{\partial R_3}{\partial v_i} = \frac{\partial g}{\partial h_i}\frac{\partial h_i}{\partial v_i}]_{P_i} + \frac{\partial g}{\partial T_i}\frac{\partial T_i}{\partial v_i}]_{P_i}$$

$$\frac{\partial g}{\partial h_i} = \dot{m}_i$$

note also that

$$\left.\frac{\partial h_i}{\partial P_i}(P_i, v_i)\right|_{v_i} \qquad \text{and} \qquad \left.\frac{\partial h_i}{\partial v_i}(p_i, v_i)\right|_{p_i}$$

are constitutive relations of the working substance and would exist as subroutines external to the [K'] system, evaluated when called for during the assembly operation. This applies as well for

$$\left.\frac{\partial T_i}{\partial P_i}\right|_{v_i} \qquad \text{and} \qquad \left.\frac{\partial T_i}{\partial v_i}\right|_{P_i}$$

The function $\partial g/\partial T_i$ shall be evaluated numerically to avoid the analytical function involving the logarithm. In general, the numerical derivative for a function of multiple variables with respect to the variable x_i is

$$\frac{\partial g(x_1, x_2, \ldots, x_i, \ldots, x_n)}{\partial x_i} = \frac{g(x_1, x_2, \ldots, x_i + \Delta x_i, \ldots, x_n) - g(x_1, x_2, \ldots, x_i, \ldots, x_n)}{\Delta x_i}$$

For this numerical representation, the contribution to the linearization function from the $\dot{m}_i h_i$ terms subtract to zero since h is not an explicit function of T in this postulation. This leaves only the non-linear (logarithmic) portion of the rate equation to be evaluated, denoted $f(T_i)$:

$$f(T_i) = U_r A_r \ln\left\{\frac{(T_1 - T_4) - (T_2 - T_3)}{(T_1 - T_4)/(T_2 - T_3)}\right\}$$

The partial derivative of the rate equation residual with respect to (say) P_1 is

$$\frac{\partial R_3}{\partial P_1} = \frac{f(T_i)}{\partial P_i} = \frac{f(T_1(P_1 + \Delta P_1, v_1), T_2, T_3, T_4) - f(T_1(P_1, v_1), T_2, T_3, T_4)}{\Delta P_1}$$

Other partial derivatives are straight forward.

The partial derivative relations for the ambient heat exchangers are similar to the results for the regenerative heat exchangers with the expected variable and parameter substitutions.

Expansion valve characteristic equation:

$$R_1 = h_1(P_1, v_1) - h_2(P_2, v_2)$$

The partial derivatives are straight forward:

$$\frac{\partial R_1}{\partial P_1} = \frac{\partial h_1}{\partial P_1}\Big]_{v_1} \qquad \frac{\partial R_1}{\partial v_1} = \frac{\partial h_1}{\partial v_1}\Big]_{P_1}$$

$$\frac{\partial R_1}{\partial P_2} = -\frac{\partial h_2}{\partial P_2}\Big]_{v_2} \qquad \frac{\partial R_1}{\partial v_2} = -\frac{\partial h_2}{\partial v_2}\Big]_{P_2}$$

Mass continuity relations.

$$\dot{m}_i - \dot{m}_{i+1} = 0$$

Since $\dot{m}_i$ are independent variables,

$$\frac{\partial R}{\partial P_i} = \frac{\partial R}{\partial v_i} \equiv 0$$

$$\frac{\partial R}{\partial \dot{m}_i} = \begin{Bmatrix} +1(\text{in-flow}) \\ -1(\text{out-flow}) \end{Bmatrix}$$

Appendix 3 Recursive Relations for Generation of the [K^t] Matrix

The partial derivatives of Section 6.2 are combined with the topology matrices to form the inner matrices, which are then used to generate the global [K^t] matrix. Each row within an inner matrix corresponds to a partial derivative of a constitutive relation for a storage element.

The recursives for the 1st law interactions are :

$$(K_{ij}^t)_p^1 = \dot{m}_j \frac{\partial h_j}{\partial P_j}\bigg|_{v_j} \mathrm{Top}_T[i,j]$$

$$(K_{ij}^t)_v^1 = \dot{m}_j \frac{\partial h_j}{\partial v_j}\bigg|_{P_j} \mathrm{Top}_T[i,j]$$

$$(K_{ij}^t)_{\dot{m}}^1 = h_j \mathrm{Top}_T[i,j]$$

The recursive relations for the characteristic equations are not uniform between the different devices. For the work transfer devices,

$$(K_{1j}^t)_P^T = \mathrm{Top}_T[i,j]\,\{\frac{\partial h_j}{\partial P_j}]_{v_j} - \eta_t\{\frac{\partial h_{js}}{\partial P_j}]_{v_j} + \frac{\partial h_{j+\mathrm{Top}_T[i,j]}}{\partial s_{j+\mathrm{Top}_T[i,j]}}]_{P_{j+\mathrm{Top}_T[i,j]}} \frac{\partial s_{j+\mathrm{Top}_T[i,j]}}{\partial P_j}]_{v_j}\}\,\{\mathrm{Top}_T[i,j]+1\}\}$$

Referring to Section 4.3, the recursion for the compressor engine is logically extended by replacing $\left(\frac{1}{\eta_t}-1\right)$ with $(1-\eta_c)$.

For the expansion valve, the temperature characteristic recursion is

$$(K_{ij}^t)_P^T = \frac{\partial h_j}{\partial P_j}\bigg|_{v_j} \text{Top}_T[i,j]$$

$$(K_{ij}^t)_v^T = \frac{\partial h_j}{\partial v_j}\bigg|_{P_j} \text{Top}_T[i,j]$$

$$(K_{ij}^t)_{\dot{m}}^T \equiv 0$$

For the regenerative heat exchanger, the partial derivative of the temperature characteristics become

$$(K_{ij}^t)_{\dot{m}}^T = h_j \text{Top}_T[i,j]$$

$$(K_{ij}^t)_P^T = \frac{\partial f(T_i)}{\partial P_j}\bigg|_{v_j} \text{Top}_T[i,j]$$

where $\frac{\partial f(T_i)}{\partial P_j}$ is the numerical derivative defined in Appendix 1. $\frac{\partial f(T_i)}{\partial P_j}$ exists as a subroutine with standard arguments ($T(P_i, v_i)$). When the topological argument is non-zero, the corresponding nodal variable will be passed to the subroutine computing the derivative and appropriately incremented (ΔP_i, or Δv_i) in both the logarithmic function in the numerator and in the denominator. Similarly,

$$(K_{ij}^t)_v^T = \frac{\partial f(T_i)}{\partial v_j}\bigg|_{P_j} \text{Top}_T[i,j]$$

Here again, the thermal topology is used.

Pressure characteristic recursions are generated by combining the partial derivatives in Appendix 1 with the *mass* topology. The pressure relations for work transfer devices require some modification to the constitutive relation to make it compatible as a numerically generated partial derivative. For pressure elevating devices, the pressure elevation is always specified on the outlet term, which indicates that indicates that K^t_{ij} must be able to distinguish inlet from outlet. This information lies in the topology matrix where all exiting flows have arithmatic value (-1). To implement this, the pressure residual must be re-arranged as follows:

$$R_1 = P_1 - r_E P_2 = 0$$

$$R_1 = \frac{1}{\sqrt{r_E}} P_1 - \sqrt{r_E} P_2$$

$$= (\sqrt{r_E})^{-1} P_1 - (\sqrt{r_E})^{+1} P_2$$

$$= r_E^{-\frac{1}{2}} P_1 - r_E^{\frac{1}{2}} P_2$$

$$= r_E^{-\frac{1}{2}\mathrm{Top}_m[i,j]} P_1 - r_E^{\frac{1}{2}\mathrm{Top}_m[i,j]} P_2$$

$$\therefore \quad \frac{\partial R_1}{\partial P_1} = \left\{ r_E^{-\frac{1}{2}\mathrm{Top}_m[1,1]} \right\} \mathrm{Top}_m[1,1] = (K'_{11})^P_m$$

and $$\frac{\partial R_1}{\partial P_2} = \left\{ r_E^{-\frac{1}{2}\mathrm{Top}_m[1,2]} \right\} \mathrm{Top}_m[1,2] = (K_{12}^t)_p^P$$

The recursive relation for a pressure characteristic can be generalized to

$$(K_{ij}^t)_p^P = \left\{ r_E^{-\frac{1}{2}\mathrm{Top}_m[i,j]} \right\} \mathrm{Top}_m[i,j]$$

Application to compression devices is simply extended by replacing r_E with r_C. The recursions for pressure characteristics experiencing momentum losses are

$$(K_{ij}^t)_p^P = \mathrm{Top}_m[i,j]$$

$$(K_{ij}^t)_m^P = \left\{ \left(\frac{-32fl}{\pi D^3} \right) \dot{m}_j (v_j + v_{j+1}) \right\} \mathrm{Top}_m[i,j]$$

$$(K_{ij}^t)_v^P = \left\{ \left(\frac{-16fl}{\pi D^3} \right) \dot{m}_j^2 (1 + v_{j+\mathrm{Top}_m[i,j]}) \right\} \mathrm{Top}_m[i,j]$$

The mass topology matrix is used to modify the variable index on the specific volume so that the recursion will generate the exact function. Section 6.3 showed that when

$$R = P_1 - P_2 - \left(\frac{16fl}{\pi D^3} \right) (\dot{m}_1^2 (v_1 + v_2)$$

$$\frac{\partial R}{\partial v_2} = \left(\frac{-16fl}{\pi D^3} \right) \dot{m}_1^2 (1 + v_1)$$

The variable index "2", which is the linearizing variable, disappears, but the variable index "1" remains. The matrix variable index is j=2, so j=2 must be modified to ensure that the variable index "1" appears in the function. This is done by using the arithmatic value of the mass topology matrix to mod fy the variable index since v_2(an outlet variable) has arithmatic value (-1).

Finally, the mass continuity interaction region can be developed. Clearly,

$$(K_{ij}^{t})_{P}^{\dot{m}} = (K_{ij}^{t})_{v}^{\dot{m}} \equiv 0$$

The mass flux partial derivative for the continuity interaction are identically the mass topology matrix:

$$(K_{ij}^{t})_{m}^{\dot{m}} = \mathrm{Top}_{m}[i,j]$$

where "i" corresponds to a mass continuity constitutive relation.

Appendix 4 Appendix 4: Numerical Solution of $[K^t(x_i)]\{\Delta x\}=\{R(x_i)\}$

Numerical solution (or reduction) of the $[K^t(x_i^k)]\{\Delta x^k\}=\{R(x_i^k)\}=0$ system is accomplished using a Newton-Raphson scheme. The index "k" represents the "kth" numerical value based on thermodynamic state $\{x^k\}$. The reduction operation consists of an initial estimate to the independent variable vector $\{x^0\}$. $\{x^0\}$ is then used to assign a numerical value to $[K^t(x^0)]$). The product $[K^{t,0}]\{\Delta x^0\}$ is formed which is the first estimate for the system's constitutive relations. The same value of $\{x^0\}$ is used to compute the residual relations $\{R(x^0)\}$, which is then compared to $\{\varepsilon\}$, the error vector. Typically, $\{R(x^0)\}>\{\varepsilon\}$, which requires modifying (iterating) the vector $\{x\}$ until $\{R(x^0)\}<\{\varepsilon\}$.

The $\{x\}$ vector is initialized to $\{x^0\}$ by the user based on some educated or experience-based guess. When $\{x^0\}$ is established, $[K^t(x)]$ assumes its first numerical approximation, $[K^{t,0}]$. Each time the $\{R(x^k)\}$ exceeds the error vector $\{\varepsilon\}$, $\{x\}$ can be updated by

$$\{x^{k+1}\} = -[K^t(x^k)]^{-1}\{R(x^k)\} + \{x^k\}$$

$$\{x^{k+1}\} = \{\Delta x^k\} + \{x^k\}$$

This is simply Newton's Method solved for $\{x^{k+1}\}$, the improved estimate.

The error vector $\{\varepsilon\}$ is used to check for convergence toward the equilibrium state $\{x^{eq}\}$ by comparison with the $\{R(x^k)\}$. Therefore, $\{\varepsilon\}$ should reflect the scale of the constitutive relation to which it refers. If $\{\varepsilon\}$ is suitably chosen, it will ensure quick convergence with acceptable accuracy; $\{\varepsilon\}$ too large will yield rapid convergence but poor accuracy while

on the other hand $\{\varepsilon\}$ too small will lead to longer convergence times while generating accuracy that may be excessive for the needs of the analysis. The method proven useful in Dr. Russo's CAT methodology is to use a fractional error based on the constitutive relation of interest:

$$\varepsilon_i = \frac{|R_i(x^0)|}{n}$$

where "n" represents the number of independent variables. For a small system, n may be too small to render desired accuracy, in which case some other suitable divisor may be used. This is a proven, simple and consistent system scaling technique.

When $\{x^{eq}\}$ is attained, the post processing calculations are executed since all the independent variables are known and all the post-processing relations are functions of the independent variables. As a minimum, the 1st Law relations for non-zero heat and work transfer are computed to complete the system analysis. Additional computations based on the now determined state variables may now be conducted as specified by the designer/operator.