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Program CYCLE: A Rankine Cycle Analysis Routine

J. P. Abbin and W. R. Leuenberger

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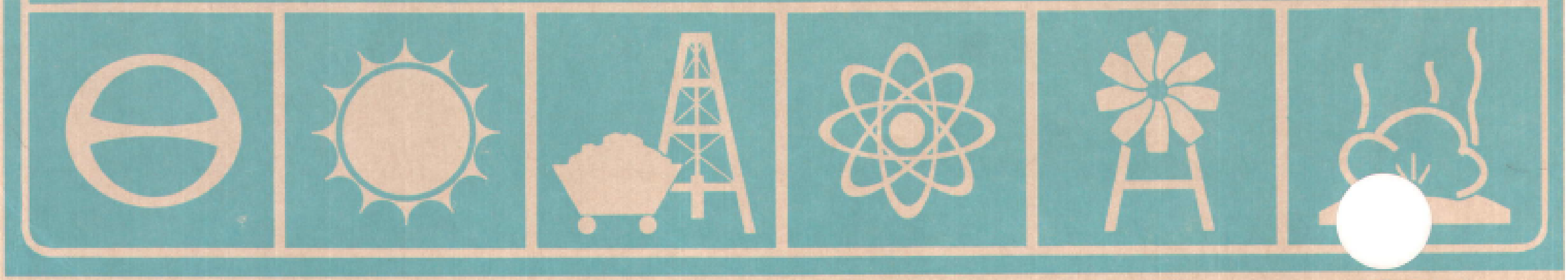

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PROGRAM CYCLE: A RANKINE CYCLE ANALYSIS ROUTINE

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ABSTRACT

This report describes the computer program CYCLE which models and analyzes various Rankine cycle systems including supercritical cycles with or without regeneration and subcritical cycles with or without regeneration and/or super heat. The program will accommodate a variety of working fluids, generating the required thermodynamic properties internally using a modest number of input constants. The program version presented in this report is written in Fortran IV in a conversational mode suitable for timesharing.

ACKNOWLEDGMENT

Sincere thanks to Dr. David R. Miller of the Monsanto Research Laboratory whose work and suggestions were invaluable in the preparation of program CYCLE.

Also many thanks to Calvin B. Rogers, Photovoltaic Systems Definition Project Division 5719, Sandia Laboratories, who corrected several errors and suggested several improvements to CYCLE. Mr. Rogers also converted CYCLE to run on Sandia's CDC 6600 NOS computing system.

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LIST OF SYMBOLS

A - area, ft^2

a - Helmholtz function, $a = u - Ts$

C - specific heat, BTU/lb_m °Rankine

c - velocity ft/sec

D - specific diameter, $\left[(sec^2 * lb_f)/(ft * lb_m)\right]^{.25}$

E - efficiency

g - gravitational constant, 32.174 $lb_m * ft/lb_f * sec^2$

h - specific enthalpy, BTU/lb_m

J - Joule's constant, 777.649 $ft * lb_f/BTU$

$\dot{m}$ - mass flow, lb_m/sec

M - molecular weight, lb-moles

N - specific speed, $\left[(ft * lb_m)/(lb_f * sec^2)\right]^{.75}$

P - pressure, lb_f/in^2 or lb_f/ft^2

p - $\left(\frac{\text{pressure}}{\text{critical pressure}}\right)$

Q - heat quantity, BTU

$\dot{Q}$ - heat rate, BTU/sec

R - gas constant, 1545. $ft * lb_f/lb$ - mole * °Rankine

s - specific entropy, BTU/lb_m °Rankine

T - temperature, °Rankine

t - $\left(\frac{\text{temperature}}{\text{critical temperature}}\right)$

u - specific internal energy, BTU/lb_m

V - volume, ft^3

$\dot{V}$ - volumetric flow rate, ft^3/sec

v - specific vol, ft^3/lb_m

$\dot{W}$ - power, $ft\text{-}lb_f/sec$

Z - compressibility factor, PV/MRT

$\left.\begin{matrix}CP0\\CP1\\CP2\end{matrix}\right\}$ - constants for vapor constant pressure specific heat

LIST OF SYMBOLS (Cont)

$\left.\begin{array}{l}\mathrm{CPL0}\\ \mathrm{CPL1}\\ \mathrm{CPL2}\end{array}\right\}$ - constants for liquid constant pressure specific heat

$\left.\begin{array}{l}K_o\\ \alpha\\ \beta\\ \mathrm{AR1}\\ \mathrm{AR2}\\ \mathrm{AR3}\\ \mathrm{AR4}\\ \mathrm{AW1}\\ \mathrm{AW2}\\ \mathrm{COPH1}\\ \mathrm{COPH2}\end{array}\right\}$ - constants for Hirschfelder, Buehler, McGee, and Sutton (HBMS) equation of state

ρ - density, lb_m/ft^3

ϕ - $\frac{\text{density}}{\text{critical density}}$

FTR - error function

FROJ - difference between constant pressure and constant volume specific heats $[C_p(\rho, T) - C_v(\rho, T)]$

Subscripts

b - boiling

C - condenser

c - at critical point

g - gas or vapor

G - generator

l - liquid

n - nozzle

P - pump

p - constant pressure

r - regenerator

s - constant entropy

T - turbine or prime mover

t - constant temperature

v - constant volume

vp - vapor pressure

ρ - constant density or specific volume

τ - nozzle throat

1, 2, 3, 4, ... - state points

PROGRAM CYCLE: A RANKINE CYCLE ANALYSIS ROUTINE

I. Introduction

A major part of Sandia's Solar Community[1] effort involves a computer study which will analyze and evaluate systems for the conversion of solar energy to provide the community's total energy needs. Because of the large number and the complexity of the subsystems involved, a master computer program is being written[2] to describe and compare alternate systems. As described in Reference 2, the master program, SOLSYS, incorporates subroutines for describing solar input, weather data, community heating, cooling, and electrical loads, and the numerous subsystems such as the collectors, heat storage, etc. The baseline solar-to-electrical conversion system for the Solar Community is the Rankine cycle which was chosen as a result of studies by Sandia[3] and others[4] which indicate that this system would yield the most power per dollar of the presently available solar conversion options. This report describes a computer subroutine which is used to model a Rankine cycle power conversion system. The subroutine is presently operational on Sandia's CDC 6600 computer as part of program SOLSYS and as a main program, CYCLE, on the NOS time sharing computer system.

A simple Rankine cycle system schematic is shown in Figure 1-1. Such a system uses a working fluid vapor taken from a boiler at elevated temperature and pressure and expanded through a prime mover to produce work and/or electricity. The expanded low pressure vapor is then condensed to a liquid and pumped back to the boiler where it is revaporized in a continuous process.

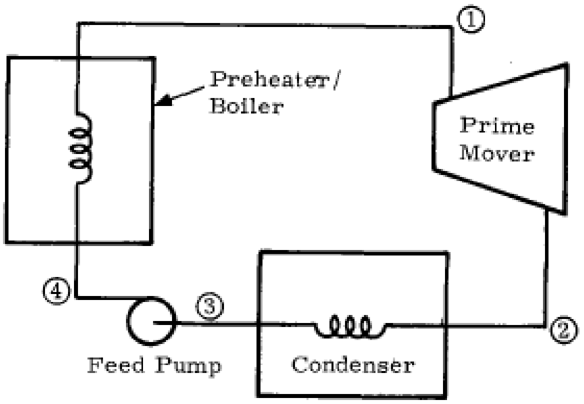


Figure 1-1. Schematic of a simple Rankine cycle system.

With the proper choice of components, particularly the working fluid, the Rankine cycle can be made to operate at efficiencies of 50 percent or greater of the Carnot (most efficient heat cycle) efficiency over a broad range of temperatures. The thermodynamic properties of the working fluid inherently contribute to the maximum possible theoretical efficiency of the cycle and these thermodynamic properties along with other physical properties of the fluid determine the type and efficiency of component hardware required.

One of the most useful tools for visualizing and analyzing the Rankine cycle is a temperature-entropy (T-s) chart. Such a chart for water is shown in Figure 1-2. Water is by far the most common Rankine cycle working fluid and is currently being used in all major electrical power plants. Water has many advantages: low cost, nonflammable, nontoxic, etc. Unfortunately, water has several disadvantages from a thermodynamic point of view as we shall see. Referring back to the diagram of a simple Rankine cycle in Figure 1-1 and labeling the corresponding points in Figure 1-2 for an ideal Rankine cycle using water we get the cycle shown by the solid line. We have an isentropic (reversible, adiabatic) expansion through the prime mover from P_1 and T_1 to P_2 and T_2 between points 1 and 2, a constant pressure and constant temperature heat rejection in the condenser between points 2 and 3, an isentropic pumping process from P_2 to P_1 between points 3 and 4, a constant pressure heating process of the liquid from T_4 to T_1 between points 4 and 4a, and finally a constant pressure and temperature heat addition (boiling) process between points 4a and 1. The net work and rejected heat are represented by the labeled areas on the chart. The overall efficiency is given by

$$E = \frac{\text{Net Work}}{\text{Input Heat}} = \frac{\text{Net Work}}{\text{Net Work + Rejected Heat}} .$$

Note that the Efficiency will be a maximum for any given high and low temperature combination if the net work area is a rectangle on the T-s diagram as shown in Figure 1-3. This cycle is the ideal Carnot cycle which is the basis of comparison for all heat cycles but which is not a realizable cycle for many reasons.[5] The efficiency of the ideal Carnot cycle is given by

$$E_{\text{Carnot}} = \frac{T_{\text{high}} - T_{\text{low}}}{T_{\text{high}}} .$$

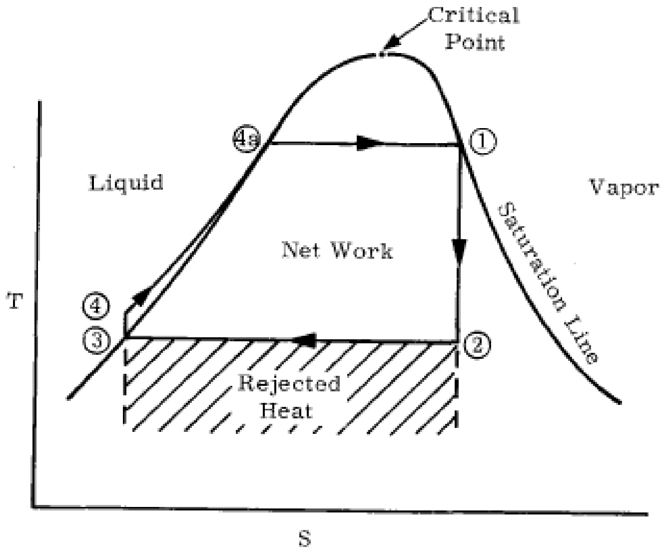
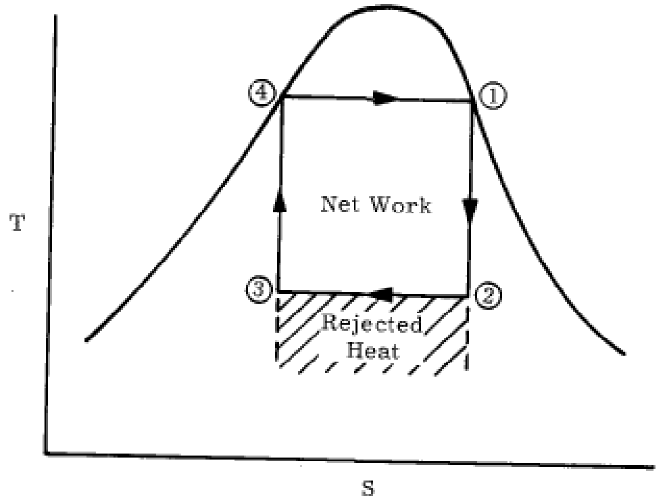


Figure 1-2. Temperature vs. entropy diagram for water with a simple Rankine cycle superimposed.

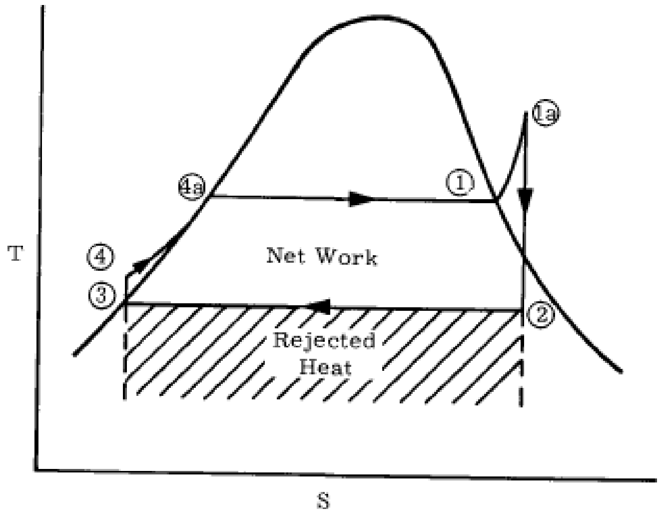
Figure 1-3. Temperature vs. entropy diagram for water with a Carnot cycle superimposed.



Referring back to Figure 1-2, note that the expansion from 1 to 2 results in a mixture of vapor and liquid (wet vapor) at 2. Fluids such as water with a negative slope for the saturated vapor line are thus called "wetting" fluids because of the above characteristic. Wet vapor is undesirable in a turbine because it causes blade erosion and lower efficiency since the liquid droplet velocity lags behind the average vapor stream velocity and impinges on the backside of the blades. Positive displacement machines must also provide for removal of this moisture to prevent water from accumulating and damaging the machine.

To overcome this problem with wetting fluids, superheating is employed as shown in Figure 1-4. Heat is added at constant pressure (ideally) such that the wet vapor region is not penetrated excessively at the end of the expansion. A quick look at Figure 1-4 and the relative net work vs. rejected heat area indicates, however, that this cycle is thermodynamically less efficient than those shown in Figures 1-2 and 1-3 if the high and low temperatures are the same for all cycles.

Figure 1-4. Temperature vs. entropy diagram for water with a superheat Rankine cycle superimposed.



With the above and other considerations in mind, we could propose an ideal Rankine cycle working fluid[5] with the following properties:

1) The heat capacity of the liquid phase should be small. This would mean the line 4-4a in Figure 1-2 would become more vertical.

2) The critical point should be above the highest operating temperature to allow all the heat to be added at the high temperature. This can be a disadvantage in transferring the heat to the working fluid from a heat source which is only slightly hotter than hottest working fluid such as that from a solar collector or nuclear reactor.

3) The vapor pressure at the highest operating temperature should be moderate (e. g., 1000 psia or less) for safety reasons and to minimize pump work and equipment cost.

4) The vapor pressure, P_2 at the condensing temperature, T_2, should not be lower than atmospheric to prevent air leakage into the system which would prevent expanding down to the saturation pressure of the working fluid at T_3.

5) The specific vapor volume, at the condensing temperature should be small to avoid large diameter turbine wheels (large blades), casings, and heat exchangers.

6) The fluid should be a liquid at atmospheric pressure and temperature for ease of handling and containment.

7) The saturated vapor line on the T-s chart should be vertical to avoid expansion into the wet vapor region (negative $\frac{dT}{ds}$ slope) or expansion into the superheat region (positive $\frac{dT}{ds}$ slope).

8) For low power turbine applications, the fluid should have a high molecular weight to minimize the rotational speed and/or the number of turbine stages and to allow reasonable mass flow rates and nozzle areas.

9) The fluid should have good heat transfer properties, be inexpensive, stable at the highest desired operating temperature, nonflammable, noncorrosive, nontoxic, etc.

Figure 1-5 illustrates some of these characteristics and graphically shows how a Carnot cycle could theoretically be approached.

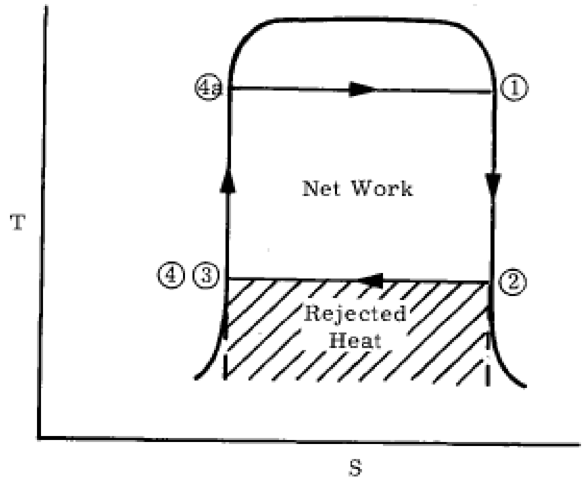


Figure 1-5. Temperature vs. entropy diagram for an ideal Rankine cycle working fluid with a simple Rankine cycle superimposed.

No single fluid can provide all of the desired characteristics for a given application, but it is possible to find a fluid which gives superior performance.

Many authors have investigated the fluid selection problem,[6,7,8] and it appears that for maximum operating temperatures less than 600°F, there are a multitude of working fluid candidates. The hydrocarbon family, due to its sheer size, offers the greatest number of fluids from which to select.

An example of a hydrocarbon working fluid is toluene, C_7H_8, a relatively common industrial chemical used primarily as a solvent. The T-s diagram for toluene is shown in Figure 1-6. As can be seen in the T-s diagram, toluene is a "drying" type fluid which emerges superheated after expansion through a prime mover. This superheat would be lost in the condenser if we did not add a "regenerator" (heat exchanger) to transfer as much of the superheat as possible to the liquid going to the boiler. A schematic of a regenerative Rankine cycle is shown in Figure 1-7, and the corresponding state points are shown in Figure 1-6.

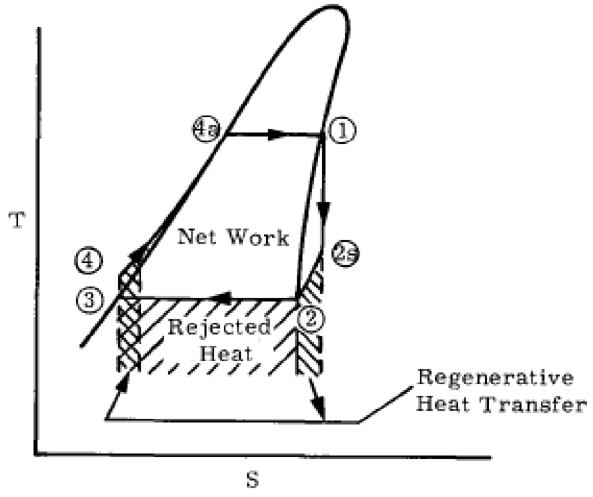


Figure 1-6. Temperature vs. entropy diagram for toluene with an ideal regenerative Rankine cycle superimposed.

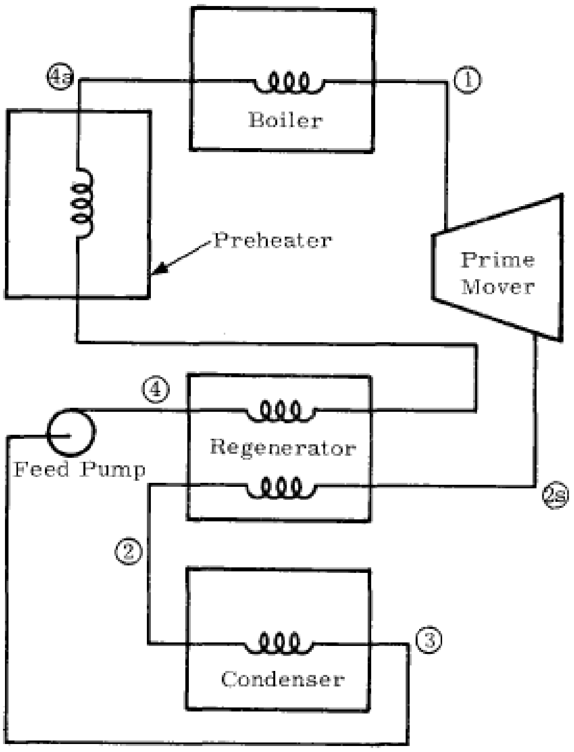


Figure 1-7. Schematic of a regenerative Rankine cycle system.

The subject program analyzes both simple and regenerative supercritical, subcritical, and subcritical with superheat Rankine cycles operating with any type ("wetting", "drying", isentropic) working fluid.

All fluid property calculations in the gaseous phase are accomplished by the use of the Hirschfelder-Buehler-McGee-Sutton (HBMS) equation of state.[9] This equation has the capability of accurately modeling a variety of working fluids over any temperature range for which a relatively moderate number of input constants are available. Mathias' method[10] and Benson's method[10] were combined to calculate the specific volume of the saturated liquid used in the calculation of the pump work. Heat of vaporization calculations, used for both boiler and condenser heat rates, are done with the Chen modification of the Pitzer Accentric-factor correlation equation.[10] The reduced Kirchhoff (vapor-pressure) equation[10] is used for pressure and temperature calculations along the saturated vapor line. Component efficiencies are inputed into the program at execution. The cycle analysis and the application of the above calculations are described in the following sections.

The only major limitation of this program is that cycle-fluid combinations which involve prime mover inlet and outlet state points in the wet vapor or dense gas (density greater than critical) regions cannot presently be analyzed. In most cases, the program will not allow inputs which create these conditions. Section III presents a discussion of the program's input logic which prevents calculations outside the appropriate areas and further discusses the limitations.

II. Cycle Analysis

A schematic of an example Rankine cycle analyzed by program CYCLE is shown in Figure 1-7. A corresponding T-s diagram for a "drying" type fluid and a subcritical cycle is shown in Figure 2-1. The program will handle numerous variations of the example cycle (e.g., superheat, supercritical) and other type fluids (e.g., "wetting") but the example cycle will illustrate the type of calculations involved.

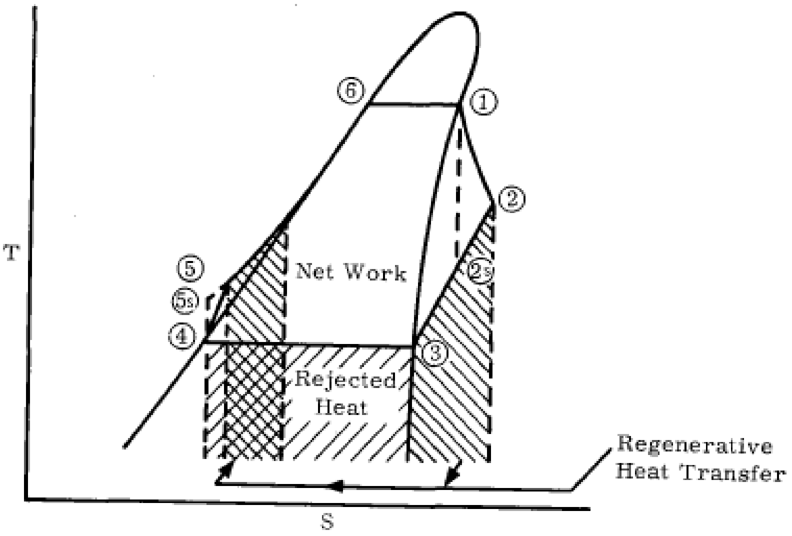


Figure 2-1. T-s diagram for a "drying" type fluid with a nonideal regenerative Rankine cycle superimposed.

The cycle shown in Figure 2-1 differs from that shown in Figure 1-6 in that the expansion process from 1 to 2 and the pumping process from 4 to 5 are no longer assumed to be ideal (isentropic). The dotted lines and the state points with the s indicate the isentropic process. The following outline for the cycle analysis as performed by CYCLE assumes all of the fluid parameters are known--the method of calculation of these parameters is given in the following Sections. Under each heading, the last equation is the form used in the program.

Net Cycle Power and Mass Flow Rate

$$\dot{W} = E_G \dot{m} \left[(h_1 - h_2) - (h_5 - h_4)\right]$$

$$= E_G \dot{m} \left[E_T (h_1 - h_{2s}) - \frac{1}{E_P} (h_{5s} - h_4)\right] . \qquad (2\text{-}1)$$

Regenerator Heat Rate (Vapor Side)

$$\begin{aligned}\dot{Q}_{rg} &= \dot{m}\,(h_2 - h_3)\\ &= \dot{m}\left[(h_2 - h_{2s}) - (h_{2s} - h_3)\right]\\ &= \dot{m}\left[(h_1 - h_{2s})(1 - E_T) - (h_{2s} - h_3)\right] \;. \qquad (2\text{-}2)\end{aligned}$$

Regenerator Heat Flow Rate (Liquid Side)

$$\dot{Q}_{rl} = E_r \dot{Q}_{rg} \;. \qquad (2\text{-}3)$$

Total Input Heat Rate (No Regeneration)

$$\begin{aligned}\dot{Q} &= \dot{m}\,(h_1 - h_5)\\ &= \dot{m}\left[(h_1 - h_6) + (h_6 - h_4) - (h_5 - h_4)\right]\\ &= \dot{m}\left[(h_1 - h_6) + (h_6 - h_4) - \frac{1}{E_P}(h_{5s} - h_4)\right] \;. \qquad (2\text{-}4)\end{aligned}$$

For superheat cycles, there is an additional term for the superheat. For supercritical cycles, the input heat rate is calculated from the sum of the output heat rates less the pump work, i.e.

$$\begin{aligned}\dot{Q} &= \dot{m}\left[(h_1 - h_2) + (h_2 - h_3) + (h_3 - h_4) - (h_5 - h_4)\right]\\ &= \dot{m}\left[(h_1 - h_{2s}) + (h_{2s} - h_3) + (h_3 - h_4) - \frac{1}{E_P}(h_{5s} - h_4)\right] \;. \qquad (2\text{-}5)\end{aligned}$$

Total Input Heat Rate (With Regeneration)

$$\dot{Q}(\text{with regeneration}) = \dot{Q} - \dot{Q}_{rl} \;. \qquad (2\text{-}6)$$

Condenser Heat Rate (With Regeneration)

$$\dot{Q}_C = \dot{m}\,(h_3 - h_4) + (1 - E_r)\dot{Q}_{rg} \;. \qquad (2\text{-}7)$$

Overall Efficiency (No Regeneration)

$$E = \frac{W}{\dot{Q}} \;. \qquad (2\text{-}8)$$

Overall Efficiency (With Regeneration)

$$E(\text{with regeneration}) = \frac{W}{\dot{Q}\ (\text{with regeneration})} \quad . \tag{2-9}$$

In addition to the above, several other quantities of lesser importance, which are primarily of interest for component design, are calculated by CYCLE. The nozzle throat and exit areas, the nozzle spouting velocity, the turbine exhaust flow rate, the turbine specific speed, and the turbine specific diameter are calculated for a single stage impulse turbine. This type of prime mover is a logical candidate for relatively low power applications such as anticipated for initial experimentation for the Solar Community. The quantities listed above give an indication as to the practicality of a single stage impulse turbine for the cycle being analyzed. The boiler feed pump horsepower, volumetric flow rate, pressure differential, and the lower operating temperature essentially define the requirements on the feed pump. The above quantities are calculated using the equations which follow.

Nozzle Spouting (Exit) Velocity

$$c_2 = \frac{E_n \sqrt{2gJ(h_1 - h_{2s})}}{\left[1 - \left(\frac{\rho_2 A_2}{\rho_1 A_1}\right)^2\right]} \tag{2-10}$$

Nozzle Throat and Exit Areas

$$A_\tau = \frac{\dot{m}}{E_n \rho_\tau c_\tau} \tag{2-11}$$

$$A_2 = \frac{\dot{m}}{\rho_2 c_2} \quad . \tag{2-12}$$

Turbine Exhaust Flow

$$\dot{V}_T = \dot{m} v_2$$

$$= 60\, \dot{m} v_2 \ \text{ft}^3/\text{minute}. \tag{2-13}$$

Feed Pump Power

$$W_P = \dot{m}\,(h_5 - h_4)$$

$$= \dot{m}\,\frac{v_1}{E_P}\,(P_1 - P_2)$$

$$= \dot{m}\,\frac{v_1}{E_P}\,(P_1 - P_2)\left(\frac{144}{550}\right)\ \text{hp}\ . \qquad (2\text{-}14)$$

Feed Pump Volumetric Flow

$$\dot{V}_P = \dot{m}v_1\ . \qquad (2\text{-}15)$$

Turbine Specific Speed (for a single stage impulse turbine rotor diameter of one foot and a rotor tip velocity equal to one half the nozzle spouting velocity)

$$N_T = \frac{60(c_2/2)\sqrt{\dot{V}_T/60}}{3.1416\left[J(h_1 - h_{2s})\right]^{.75}}\ . \qquad (2\text{-}16)$$

Turbine Specific Diameter (for a turbine rotor diameter of one foot)

$$D_T = \frac{\left[J(h_1 - h_{2s})\right]^{.25}}{\sqrt{\dot{V}_T/60}}\ . \qquad (2\text{-}17)$$

III. Program Input Logic

Each of the different Rankine cycles this program evaluates goes through a different grouping of calculations. The program does not require the type of cycle to be inputed, since this is determined by the program logic. This logic section not only determines what type of cycle is to be evaluated but also helps the user by indicating what pressures are allowable for several of the possible cycles.

This program can evaluate five different types of cycles:

1) Subcritical drying fluid cycle with or without regeneration,
2) Subcritical wetting fluid cycle with superheat and with or without regeneration,
3) Supercritical wetting fluid cycle with or without regeneration,
4) Subcritical drying fluid cycle with superheat and with or without regeneration, and
5) Supercritical drying fluid cycle with or without regeneration.

Figure 3-1 is a flow chart which shows the logical steps involved when reaching each of these cycles. P_{calc} and P_{KCF} are used within Figure 3-1 to indicate previously calculated values and values calculated along the saturated vapor line with Kirchoff's equation, respectively.

For all cycles, the fluid constants and high and low temperatures are inputed. The slope of the saturated vapor curve is then calculated at the average temperature, or, if the high temperature is above the critical temperature, at the average of the low and critical temperatures. As shown on the flow chart, the first check is made to see if the high temperature is above or below some operating temperature (T_{OPR}). All cycles with their high temperature below T_{OPR} are subcritical cycles. This operating temperature is defined as 95 percent of the critical temperature and is used instead of the critical temperature because some subcritical drying fluid cycles cannot expand off the saturated vapor curve near the critical point without ending with a wet vapor mixture. As stated earlier, this program does not allow expansions which cross the saturated vapor line.

For the case where the input high temperature is less than the operating temperature, T_{OPR}, the next check is the slope of the saturated vapor line.

For positive slopes, we are dealing with a Type 1 or Type 4 cycle. The program then asks if the user wants to input the high pressure. Any response other than a "YES" results in a Type 1 cycle. A "YES" results in a Type 4 cycle and the program calculates the pressure on the saturated vapor line corresponding to the inputed high temperature. The program then instructs the user to enter a high pressure less than the pressure it has just calculated. For negative slopes, we are dealing with a Type 2 cycle, and the program applies the isentropic process equation from the low temperature on the saturated vapor curve to the high temperature and calculates the corresponding

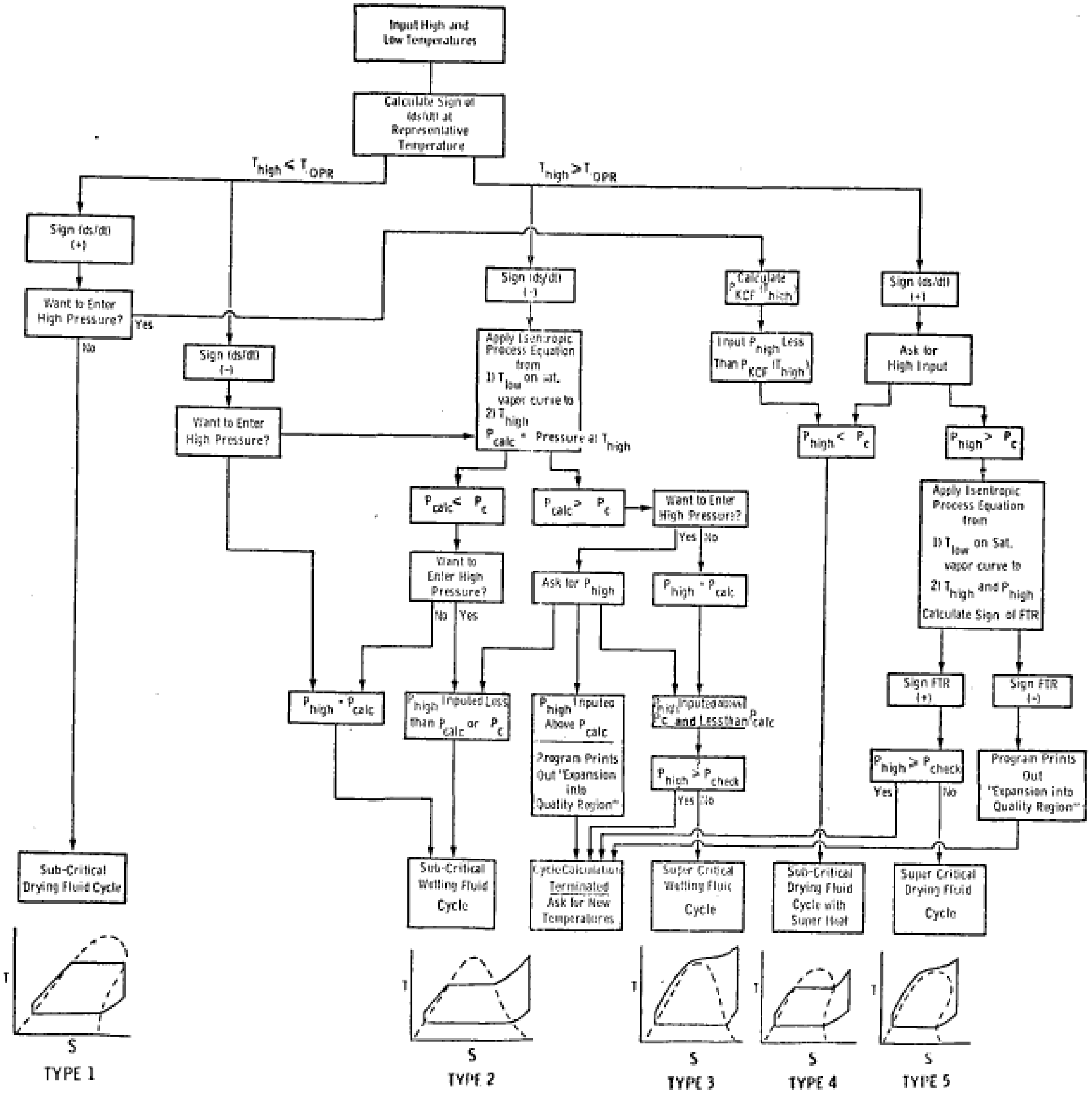


Figure 3-1. Block diagram for program input logic.

high pressure. The program now asks the user if he wants to enter the high pressure. For any answer other than a "YES", the state point just calculated is used for the prime mover input conditions, and for a "YES" answer, the program instructs the user to input a high pressure less than the one just calculated. For both answers, the user ends up with a Type 2 cycle, but with a variable amount of superheating and regeneration.

For input high temperatures above T_{OPR}, it is still possible to end up with a subcritical cycle. For the case where the high temperature is above the operating temperature and the saturated vapor curve has a negative slope (wetting fluid), the isentropic process equation is automatically applied from the low temperature point on the saturated vapor line to the high temperature. A high pressure is the result of this calculation. If this high pressure is less than the critical pressure, the program asks the user if he wants to enter the high pressure and so on as described in the previous paragraph. If the high pressure calculated with the isentropic expansion equation is greater than the critical pressure, the program also asks the user if he wants to enter the high pressure. Any answer other than "YES" results in a Type 3 cycle and the program immediately begins the cycle evaluation. For a "YES" answer, the program instructs the user to enter a pressure less than the pressure calculated with the isentropic process equation. The user can then input a pressure less than critical, resulting in a Type 2 cycle, or a pressure greater than critical but less than the calculated pressure and end up with a Type 3 cycle.

For input high temperatures greater than T_{OPR} and a positive sloping saturated vapor curve (drying fluid) the program automatically asks for a high pressure input. If this input high pressure is less than the critical pressure, a Type 4 cycle will be analyzed. If the input high pressure is above the critical pressure, the isentropic expansion process calculations are applied from the high temperature and pressure state point to a state point corresponding to the low temperature point on the saturated vapor line. For this case, the error function in the iteration procedure is evaluated and particular attention is paid to its sign. If the sign of the error is positive, the high temperature state point has a higher entropy value than the low temperature state point and the expansion is possible. If the sign of the error is negative, the high temperature state point has a lower entropy value than the low temperature state point and this expansion is not possible without lowering the pressure of the high temperature state point. The mechanics of this error function sign analysis are described in Section VI "Prime Mover Expansion Process." For the case where the expansion is possible, a Type 5 cycle is analyzed.

There are numerous other checks thoughout the logic section to keep a user from going astray. The low temperature is never allowed to be higher than the high temperature. When the program instructs a user to enter a pressure lower than an indicated pressure, it will not accept a higher pressure. The program will not accept an input pressure above P_{CHECK} (T), which is calculated along the critical density line above the critical pressure where the density is constant and the HBMS equation of state becomes a relationship of pressure in terms of temperature only.

IV. Slope of Saturated Vapor Curve

As shown in the preceding section, it is important to know the slope of the saturated vapor curve. The sign of this slope indicates whether the fluid is a wetting (negative slope) or drying (positive slope) fluid. For the derivation of the equation used in the program to calculate this slope, we start with the well known thermodynamic relationship: (p. 404, Eq. (14.7), Ref. 12)

$$dh = Tds + vdP \,. \tag{4-1}$$

Rearranging, substituting $\rho = 1/v$ and dividing through by dT we get

$$T\rho \frac{ds}{dT} = \rho \frac{dh}{dT} - \frac{dP}{dT} \,. \tag{4-2}$$

Because only two independent variables are required with a real gas, we can write

$$h = f(T, P) \tag{4-3}$$

and differentiating,

$$dh = \left(\frac{dh}{dT}\right)_p dT + \left(\frac{dh}{dP}\right)_t dP \tag{4-4}$$

dividing by dT, there follows

$$\frac{dh}{dT} = \left(\frac{dh}{dT}\right)_p + \left(\frac{dh}{dP}\right)_t \frac{dP}{dT} \,. \tag{4-5}$$

By definition

$$\left(\frac{dh}{dT}\right)_p = C_p \,. \tag{4-6}$$

Starting again with Eq. (4-1)

$$dh = Tds + vdP \tag{4-7}$$

and dividing this equation by dP and applying it to a constant temperature process, we get

$$\left(\frac{dh}{dP}\right)_t = T\left(\frac{ds}{dP}\right)_t + v \tag{4-8}$$

it is also known that (p. 342, Eq. (193c), Ref. 11)

$$\left(\frac{ds}{dP}\right)_t = -\left(\frac{dv}{dT}\right)_p \quad . \tag{4-9}$$

Substituting Eq. (4-9) into Eq. (4-8), we get

$$\left(\frac{dh}{dP}\right)_t = v - T\left(\frac{dv}{dT}\right)_p \tag{4-10}$$

and substituting Eqs. (4-6) and (4-10) into (4-5) yields

$$\frac{dh}{dT} = C_p + \left[v - T\left(\frac{dv}{dT}\right)_p\right] \frac{dP}{dT} \quad . \tag{4-11}$$

Substituting Eq. (4-11) into (4-2) yields

$$T\rho \frac{ds}{dT} = \rho C_p + \left[\rho v - T\rho\left(\frac{dv}{dT}\right)_p\right] \frac{dP}{dT} - \frac{dP}{dT} \tag{4-12}$$

which reduces to

$$T\rho \frac{ds}{dT} = \rho C_p - T\rho\left(\frac{dv}{dT}\right)_p \frac{dP}{dT} \quad . \tag{4-13}$$

Dividing through by $T\rho$, it follows that

$$\frac{ds}{dT} = \frac{C_p}{T} - \left(\frac{dv}{dT}\right)_p \frac{dP}{dT} \quad . \tag{4-14}$$

Applying the perfect gas law, we have

$$\left(\frac{dv}{dT}\right)_p = \frac{R}{P} \tag{4-15}$$

which further reduces our equation to

$$\frac{ds}{dT} = \frac{C_p}{T} - \frac{1}{T}\left(\frac{RT}{P}\frac{dP}{dT}\right) \quad . \tag{4-16}$$

The well known Clapeyron Equation[12], below, is now used to reduce the equation to the final form used in the program:

$$\frac{RT}{P}\frac{dP}{dT} = \frac{\Delta h_{\text{vaporization}}}{T} \tag{4-17}$$

Substituting Eq. (4-17) into (4-16) yields

$$\frac{ds}{dT} = \frac{1}{T}\left(C_p - \frac{\Delta h_{\text{vaporization}}}{T}\right) . \tag{4-18}$$

Within the program, C_p is calculated from input data and $\Delta h_{\text{vaporization}}$ is calculated with the Chen modification to the Pitzer accentric factor correlation.[10] The use of the perfect gas law in this derivation does not yield a precise value for ds/dT; however, Eq. (4-18) is used only to determine the type of fluid and which calculations are to be made and does not degrade the program's accuracy.

V. Calculations in the Gaseous Region

The most critical calculations in this program are those in the gaseous region. These are the superheat, regenerator, and prime mover expansion calculations. Of utmost importance in these calculations is the temperature after prime mover expansion for supercritical and subcritical with regeneration cycles. For subcritical wetting fluid cycles where the fluid is expanded down to the saturated vapor line, the superheat pressure is a critical calculation. Also required for both of the above situations is an accurate calculation of the isentropic enthalpy drop in the expansion process. Some consideration was given to entering tables of properties into the computer which the program could work with, but a different set would be required for each different fluid. It was decided that if an equation of state could be found that was accurate enough, the time, effort, and computer memory associated with handling the equation would probably be small compared with entering tables of thermodynamic data into the computer and performing calculations with these tables. In this section, a relationship is derived relating the constant pressure specific heat (C_p) to the constant volume specific heat (C_v) through the chosen equation of state. This relationship is used in the following section to obtain equations for both isentropic expansion processes and for calculating the change in enthalpy between state points in the gaseous region.

Equations of state for gases are usually classified by the number of constants required for their use. The most common is the perfect gas equation which has one constant. VanderWaal's equation and Berthelot's equation are examples of two-constant equations of state. Also, there are three-constant, four-constant, five-constant, and a number of multiconstant equations of state.[10] One of these multiconstant equations of state was highly recommended and was used in this program after it had shown itself to be of sufficient accuracy.[8] The equation is the Hirschfelder, Buehler, McGee, and Sutton (HBMS) equation of state.[9]

The HBMS equation of state is one of the more complicated equations of state and is best employed in computer calculations. The variables, pressure, temperature, and density are usually expressed in their reduced form, i.e., each variable is divided by its respective critical value. The HBMS equation of state, in its standard form, has reduced pressure expressed as a function of reduced temperature and density. Iteration procedures must be written when either density or temperature is desired, and the other two variables are known. The Newton-Raphson method is used throughout the program when iteration is required. The HBMS equation, in its standard form, is

$$\frac{p}{t} = -W_1(t)\phi^2 - W_2(t)\phi^3 + g(\phi) \qquad (5\text{-}1)$$

$$W_1(t) = K_o t^{-1} + (\beta - K_o)t^{-2} \qquad (5\text{-}2)$$

$$W_2(t) = 0.5(1 - K_o - \alpha + 2\beta)(1 - t^{-2}) \qquad (5\text{-}3)$$

$$g(\phi) = \frac{(1+\beta)^3\phi}{\beta(3\beta - 1) - (3\beta^2 - 6\beta - 1)\phi + \beta(\beta - 3)\phi^2} \;. \qquad (5\text{-}4)$$

We start by stating

$$s = f(T, v) \tag{5-5}$$

differentiating

$$ds = \left(\frac{ds}{dT}\right)_\rho dT + \left(\frac{ds}{dv}\right)_t dv \quad . \tag{5-6}$$

We also know that (p. 404. Eq. (14.6), Ref. 12)

$$du = Tds - Pdv \tag{5-7}$$

dividing by dT and applying to a constant specific volume process, we get

$$\left(\frac{du}{dT}\right)_\rho = T\left(\frac{ds}{dT}\right)_\rho \quad . \tag{5-8}$$

But, by definition

$$\left(\frac{du}{dT}\right)_\rho = C_v \tag{5-9}$$

$$\therefore \left(\frac{ds}{dT}\right)_\rho = \frac{C_v}{T} \quad . \tag{5-10}$$

Introducing the Helmholtz function $a = u - Ts$, differentiating and substituting in Eq. (5-7), we have

$$da = -Pdv - sdT \tag{5-11}$$

comparing this to the total differential

$$da = \left(\frac{da}{dv}\right)_t dv + \left(\frac{da}{dT}\right)_v dT \tag{5-12}$$

and taking the second derivative of the bracketed terms and setting the derivatives equal (see page 342 of Ref. 11 for a similar derivation) we obtain

$$\left(\frac{dP}{dT}\right)_\rho = \left(\frac{ds}{dv}\right)_t \quad . \tag{5-13}$$

Substituting Eqs. (5-10) and (5-13) into (5-6) yields

$$ds = \frac{C_v}{T}\, dT + \left(\frac{dP}{dT}\right)_\rho dv \tag{5-14}$$

equating Eqs. (4-14) and (5-14) we get

$$\frac{C_p}{T}\, dT - \left(\frac{dv}{dT}\right)_p dP = \frac{C_v}{T}\, dT + \left(\frac{dP}{dT}\right)_\rho dv \quad . \tag{5-15}$$

Solving for dT

$$dT = \frac{T\left(\frac{dv}{dT}\right)_p dP}{(C_p - C_v)} + \frac{T\left(\frac{dP}{dT}\right)_\rho dv}{(C_p - C_v)} \quad . \tag{5-16}$$

We can also write that

$$T = f(v,\ P) \tag{5-17}$$

differentiating

$$dT = \left(\frac{dT}{dP}\right)_\rho dP + \left(\frac{dT}{dv}\right)_p dv \quad . \tag{5-18}$$

Then equating Eqs. (5-16) and (5-18) we obtain

$$\left(\frac{dT}{dP}\right)_\rho = \frac{T\left(\frac{dv}{dT}\right)_p}{(C_p - C_v)} \tag{5-19}$$

rearranging, we get

$$(C_p - C_v) = T\left(\frac{dv}{dT}\right)_p \left(\frac{dP}{dT}\right)_\rho \quad . \tag{5-20}$$

Remembering that the HBMS equation of state is explicit only for pressure the right side of Eq. (5-20) will be easier to evaluate if we have only derivatives of pressure with respect to the other equation of state variables.

Given that

$$P = f(v,\ T) \tag{5-21}$$

it is also known that (p. 403, Eq. (14.2), Ref. 12)

$$\left(\frac{dP}{dv}\right)_t \left(\frac{dv}{dT}\right)_p \left(\frac{dT}{dP}\right)_\rho = -1 \quad . \tag{5-22}$$

Then

$$\left(\frac{dv}{dT}\right)_p = \frac{-\left(\frac{dP}{dT}\right)_\rho}{\left(\frac{dP}{dv}\right)_t} \tag{5-23}$$

substituting this relationship back into Eq. (5-20) and substituting $\rho = 1/v$ yields

$$C_p - C_v = \frac{T\left(\frac{dP}{dT}\right)_\rho^2}{\rho^2\left(\frac{dP}{d\rho}\right)_t} \quad . \tag{5-24}$$

Rewriting the HBMS equation of state with the constants redefined as shown on p. 33 (Equations (6-11) to (6-16))

$$\frac{p}{t} = -\left(\frac{K_o}{t} + \frac{AW1}{t^2}\right)\phi^2 - AW2\left(1 - \frac{1}{t^2}\right)\phi^3 + \frac{(AR1)(\phi)}{AR2 - (AR3)(\phi) + (AR4)(\phi^2)} \quad . \tag{5-25}$$

Multiplying through by t and differentiating the resulting equation with respect to both t and ϕ, we get the two derivatives

$$\left(\frac{dp}{dt}\right)_\rho = \frac{AW1}{t^2}\phi^2 - AW2\left(\frac{t^2 + 1}{t^2}\right)\phi^3 + \frac{(AR1)(\phi)}{AR2 - (AR3)\phi + (AR4)\phi^2} \tag{5-26}$$

and

$$\left(\frac{dp}{d\phi}\right)_t = -2\left(K_o + \frac{AW1}{t}\right)\phi - 3(AW2)\left(\frac{t^2 - 1}{t}\right)\phi^2$$

$$+ \frac{(t)(AR1)\left[AR2 - (AR4)\phi^2\right]}{\left[AR2 - (AR3)\phi + (AR4)\phi^2\right]^2} \quad . \tag{5-27}$$

These derivatives are in terms of the reduced variables. Transforming the derivatives into the proper units and substituting into Eq. (5-24) yields

$$\frac{C_p - C_v}{R} = \frac{Z_c t\left[\frac{AW1}{t^2}\phi - AW2\left(\frac{t^2+1}{t^2}\right)\phi^2 + \frac{AR1}{AR2 - (AR3)\phi + (AR4)\phi^2}\right]^2}{-2t\left(\frac{K_o}{t} + \frac{AW1}{t^2}\right)\phi - 3t(AW2)\left(\frac{t^2-1}{t^2}\right)\phi^2 + t(AR1)\frac{AR2 - (AR4)\phi^2}{\left(AR2 - (AR3)\phi + (AR4)\phi^2\right)^2}} \; . \qquad (5\text{-}28)$$

This is the equation which is used to evaluate the constant volume specific heat (C_v) of a gas as either a point value or averaged over some process range.

VI. Prime Mover Expansion Process

Two important relationships are used in modeling the prime mover expansion. The first is the isentropic process equation applied to the HBMS equation of state. This equation is used in the iteration procedure to calculate the prime mover inlet or outlet conditions, depending on which cycle is being evaluated. The isentropic process equation is also used to determine if an expansion is possible from one state point to another. The second relationship developed in this section is the equation for calculating the change in enthalpy during expansion.

For the derivation of the isentropic process equation, we start with Eq. (5-14)

$$ds = \frac{C_v}{T}\, dT + \left(\frac{dP}{dT}\right)_\rho dv \tag{5-14}$$

For a constant entropy process, ds = 0, this equation reduces to

$$-\frac{C_v}{T}\, dT = \left(\frac{dP}{dT}\right)_\rho dv \ . \tag{6-1}$$

Substituting

$$v = \frac{1}{\rho} \quad \text{and} \quad dv = -\frac{d\rho}{\rho^2}$$

we get

$$\frac{C_v}{T}\, dT = \left(\frac{dP}{dT}\right)_\rho \frac{d\rho}{\rho^2} \ . \tag{6-2}$$

The final process equation written in terms of reduced variables for compatibility with the HBMS equations is

$$\frac{1}{R}\int_t \frac{C_v dt}{t} = Z_c \int_\phi \left(\frac{dp}{dt}\right)_\rho \frac{d\phi}{\phi^2} \ . \tag{6-3}$$

In Section V, we derived the equation

$$C_p - C_v = \frac{T\left(\frac{dP}{dT}\right)_\rho^2}{\rho^2\left(\frac{dP}{d\rho}\right)_t} \ . \tag{5-24}$$

The program contains a subprogram that evaluates the average value of the right-hand side of Eq. (5-24) over a temperature range. The variable name used in the program to call this calculation is FROJ. Within the iteration procedure used to calculate the state points for the prime mover inlet and outlet each time a new guess on temperature is made, the subprogram is called to calculate a new value for FROJ. The constant volume specific heat is then calculated from

$$C_v = C_p - \mathrm{FROJ} \tag{6-4}$$

where C_p is calculated from the equation

$$C_p = \mathrm{CP0} + \mathrm{CP1} * T + \mathrm{CP2} * T^2 \quad . \tag{7-1}$$

CP0, CP1 and CP2 are fluid constants and are inputed at program execution. The left-hand side of Eq. (6-3) then becomes

$$\frac{1}{R}\int_t \frac{C_v}{t}\,dt = \frac{1}{R}\int_t \frac{(\mathrm{CP0} - \mathrm{FROJ} + \mathrm{CP1} * T + \mathrm{CP2} * T^2)}{t}\,dt \quad . \tag{6-5}$$

This integrates to

$$\frac{1}{R}\int_t \frac{C_v}{t}\,dt = \frac{\mathrm{CP0} - \mathrm{FROJ}}{R}\ln\left(\frac{t_2}{t_1}\right) + \frac{\mathrm{CP1} * T_c}{R}\left(t_2 - t_1\right)$$

$$+ \frac{\mathrm{CP2} * T_c^2}{2R}\left(t_2^2 - t_1^2\right) \quad . \tag{6-6}$$

Defining

$$\mathrm{BT1}(t) = \frac{\mathrm{CP0} - \mathrm{FROJ}}{R}\ln\,(t * T_c) + \frac{\mathrm{CP1} * T_c * t}{R} + \frac{\mathrm{CP2} * T_c^2 * t^2}{2R} \quad . \tag{6-7}$$

the integral becomes

$$\frac{1}{R}\int_t \frac{C_v}{t}\,dt = \mathrm{BT1}(t_2) - \mathrm{BT1}(t_1) \quad . \tag{6-8}$$

For the right-hand side of Eq. (6-3), we start with the HBMS equation of state for the gaseous region as presented in Section V

$$\frac{p}{t} = -W_1(t) * \phi^2 - W_2(t) * \phi^3 + g(\phi) \tag{5-1}$$

where

$$W_1(t) = K_o/t + (\beta - K_o)/t^2 \tag{5-2}$$

$$W_2(t) = 0.5(1 - K_o - \alpha + 2\beta)(1 - 1/t^2) \tag{5-3}$$

$$g(\phi) = \frac{(1+\beta)^3 * \phi}{\beta(3\beta - 1) - (3\beta^2 - 6\beta - 1) * \phi + \beta(\beta - 3) * \phi^2} \ . \tag{5-4}$$

Multiplying through by t and differentiating with respect to t, we get that

$$\left(\frac{dp}{dt}\right)_\rho = \phi^2(\beta - K_o)/t^2 - \phi^3(.5)(1 - K_o - \alpha + 2\beta)(1 + 1/t^2) + g(\phi) \tag{6-9}$$

and that

$$Z_c \int_\phi \left(\frac{dp}{dt}\right)_\rho \frac{d\phi}{\phi^2} = Z_c \int_\varphi \left[\frac{(\beta - K_o)}{t^2} - .5(1 - K_o - \alpha + 2\beta)(1 + 1/t^2)\phi + \frac{(1+\beta)^3}{\beta(3\beta - 1)\varphi - (3\beta^2 - 6\beta - 1)\phi^2 + \beta(\beta - 3)\phi^3}\right] d\phi \ . \tag{6-10}$$

In order to simplify this equation, the following definitions are made

$$AR1 = (1 + \beta)^3 \tag{6-11}$$

$$AR2 = \beta(3\beta - 1) \tag{6-12}$$

$$AR3 = (3\beta^2 - 6\beta - 1) \tag{6-13}$$

$$AR4 = \beta(\beta - 3) \tag{6-14}$$

$$AW1 = \beta - K_o \tag{6-15}$$

$$AW2 = (.5)(1 - K_o - \alpha + 2\beta) \ . \tag{6-16}$$

With these definitions, Eq. (6-10) integrates to

$$Z_c \int_{\phi} \left(\frac{dp}{dt}\right)_{\rho} \frac{d\phi}{\phi^2} = Z_c \left\{ \frac{AW1}{t^2} (\phi_2 - \phi_1) - \frac{AW2}{2} \left(1 + 1/t^2\right)\left(\phi_2^2 - \phi_1^2\right) \right.$$

$$+ AR1 \left\{ \frac{1}{2(AR2)} \left[\ln\left(\frac{\phi_2^2}{AR2 - AR3\phi_2 + AR4\phi_2^2}\right) - \ln\left(\frac{\phi_1^2}{AR2 - AR3\phi_1 + AR4\phi_1^2}\right) \right] \right.$$

$$+ \frac{2AR3}{2AR2\sqrt{4(AR2)(AR4) - AR3^2}} \left[TAN^{-1}\left(\frac{2(AR4)\phi_2 - AR3}{\sqrt{4(AR2)(AR4) - (AR3)^2}}\right) \right.$$

$$\left.\left.\left. - TAN^{-1}\left(\frac{2(AR4)\phi_1 - AR3}{\sqrt{4(AR2)(AR4) - (AR3)^2}}\right) \right] \right\} \right\} . \tag{6-17}$$

Because this equation is so long and bulky, it was broken down into several parts, each of the parts being either constants or arithmetic assignment statements. A final arithmetic assignment statement gathers all these parts back into a final equation. The individual parts are:

$$PH1(\phi) = TAN^{-1}\left(\frac{2(AR4)\phi - AR3}{\sqrt{4(AR2)(AR4) - (AR3)^2}}\right) \tag{6-18}$$

$$PH2(\phi) = \ln\left(\frac{\phi^2}{AR2 - AR3\phi + AR4\phi^2}\right) \tag{6-19}$$

$$PH3(\phi, t) = \left(\frac{AW1}{t^2}\right)\phi - \frac{AW2(t^2 + 1)}{2t^2} \phi^2 \tag{6-20}$$

$$COPH1 = \frac{AR3}{\sqrt{4(AR2)(AR4) - (AR3)^2}} \left(\frac{AR1}{AR2}\right) \tag{6-21}$$

$$COPH2 = \frac{AR1}{2(AR2)} . \tag{6-22}$$

With these definitions

$$Z_c \int_\phi \left(\frac{dp}{dt}\right)_\rho \frac{d\phi}{\phi^2} = Z_c \left\{ PH3(\phi_2, t_1) - PH3(\phi_1, t_1) \right.$$

$$\left. + COPH2\left[PH2(\phi_2) - PH2(\phi_1)\right] + COPH1\left[PH1(\phi_2) - PH1(\phi_1)\right] \right\} . \qquad (6\text{-}23)$$

Combining equations (6-3), (6-8), and (6-23) yields

$$\frac{BT1(t_2) - BT1(t_1)}{Z_c} = PH3(\phi_2, t_1) - PH3(\phi_1, t_1) + COPH2\left[PH2(\phi_2) - PH2(\phi_1)\right]$$

$$+ COPH1\left[PH1(\phi_2) - PH1(\phi_1)\right] \qquad (6\text{-}24)$$

which must be satisfied for a constant entropy process.

For our use, we have found it more desirable to define an error function and then set up the iteration procedure in such a way that we drive this error function to zero. This error function (FTR), then, becomes

$$\frac{S_2 - S_1}{-RZ_c} = FTR(t_1, t_2, \phi_1, \phi_2) = \frac{BT1(t_1) - BT1(t_2)}{Z_c} + COPH2\left[PH2(\phi_2) - PH2(\phi_1)\right]$$

$$+ COPH1\left[PH1(\phi_2) - PH1(\phi_1)\right]$$

$$+ PH3(\phi_2, t_1) - PH3(\phi_1, t_1) \; . \qquad (6\text{-}25)$$

There are three iteration procedures where this error function is used. The first is the case where prime mover inlet conditions are known and the exhaust temperature is desired. The second is where the exhaust conditions are known and the inlet pressure is desired. This second case is also used to inform the user, during program execution, what maximum pressure can be inputed for a cycle evaluation. The third case where the error function is used is in calculating the isentropic nozzle throat conditions when the turbine inlet (nozzle inlet) conditions are known.

Figure 6-1 depicts the conditions for the first case (1) iteration. The inlet pressure and temperature are known along with the condenser pressure and temperature. Because the isentropic expansion can expand only as low as the condenser pressure, the exhaust temperature is determined by the intersection of the condenser pressure line and the isentropic process line from the inlet condition. The first action in the iteration is to guess a temperature somewhere between

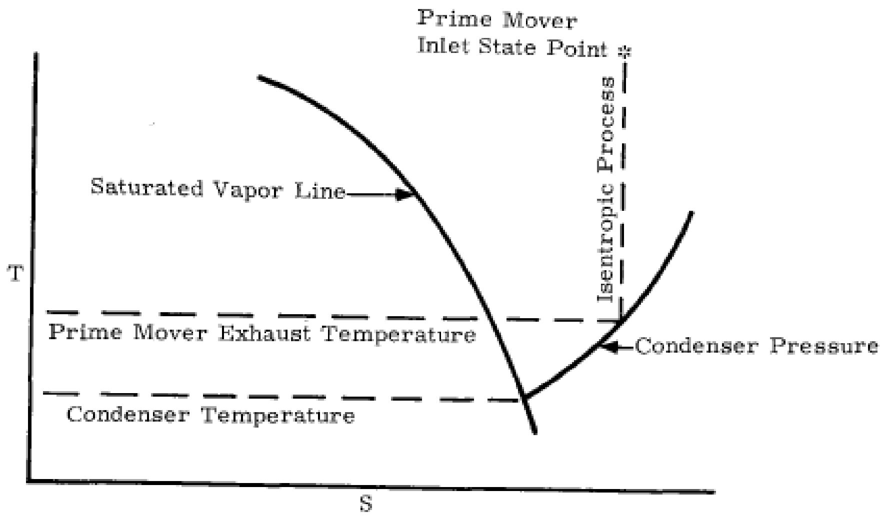


Figure 6-1. T-s diagram showing conditions for temperature after expansion iteration.

the prime mover inlet temperature and the condenser temperature. The next step is to force the error function (FTR) to zero for the assumed temperature. This yields a value of the density at the assumed temperature. For this combination of density and temperature, the pressure is calculated using the HBMS equation of state. This calculated pressure is compared with the condenser pressure, and if their difference is more than 0. 1 psia, a new temperature guess is calculated. This new temperature is calculated from an equation similar to the perfect gas polytropic process equation, and the above procedure is repeated.

Figure 6-2 depicts the conditions for the case (2) iteration. The prime mover exhaust temperature and pressure are known along with the inlet temperature. This calculation is different than the case (1) iteration in that here we know both temperatures and are calculating the inlet pressure. Knowing the two temperature extremes, the first guess of the inlet density is made with an equation similar to the perfect gas isentropic expansion equation. With the known inlet temperature and approximated density, the first guess on inlet pressure is made with the HBMS equation of state. These calculations were necessary so that the first approximation of FROJ could be evaluated. Then, using the prime mover inlet temperature and exhaust temperature and density, the isentropic error function, FTR, is forced to zero. This results in the value of the inlet density. The inlet pressure is then calculated using the density that resulted from forcing the isentropic error function to zero and the given inlet temperature. This pressure is compared with the first guess on inlet pressure, and only when the difference is less than 0. 1 psia is the program allowed to continue. Each time the difference is greater than 0. 1 psia, the first guess on inlet pressure is updated and a better value of FROJ is calculated. Actually, this calculation would be relatively easy and straightforward were it not for FROJ. The third case is discussed in Section XI.

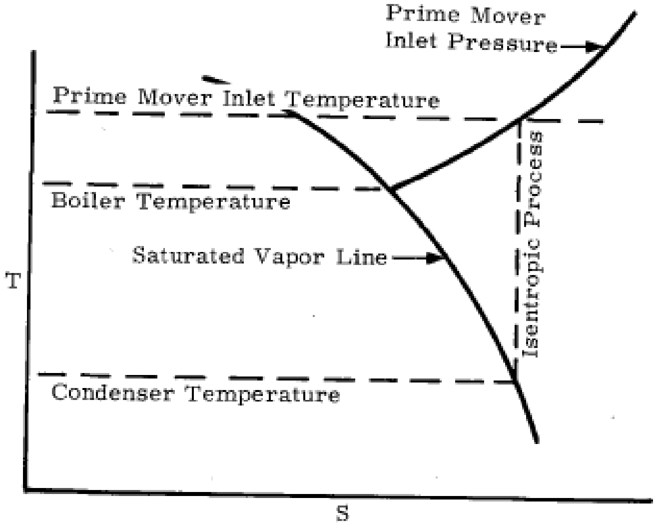


Figure 6-2. T-s diagram showing conditions for expander inlet pressure iteration.

The isentropic process, Eq. (6-25), is also used to determine if an expansion is possible between two state points. Given the two temperatures and densities, they can be inserted into this error function equation, and the value of the error calculated. As shown in Figure 6-3, the true isentropic expansion goes from point 1 to 2. The constant density line through point 3 represents a higher density than at point 2 and point 2 is a higher density than point 4. The expansion from point 1 to 3 is an expansion with a decrease in entropy and ends up at a density higher than the isentropic expansion density for that temperature. The change in density for this expansion would be smaller than for the isentropic expansion and a close look at Eq. (6-25) shows that FTR will be positive for this case. For the other case, expansion from point 1 to 4, FTR will be negative. The only time this calculation is used in the program is for supercritical drying fluid cycles. For this case, after the high and low temperatures are inputed, a high pressure is asked for. The low pressure is calculated on the saturated vapor line. FTR is then evaluated between these two state points. If FTR, evaluated between these two points, is negative, an isentropic expansion between these two temperatures can occur only if the inlet pressure is reduced or if the expansion goes into the quality region. Because the program has already accepted the high pressure, it prints out that the expansion goes into a quality region, terminates that cycle calculation, then asks if another cycle is to be evaluated.

The second relationship to be generated in this section is the equation for calculating the change in enthalpy for the prime mover expansion. As with the isentropic process equation, we will first show the derivation of the process equation, then apply it to the HBMS equation of state.

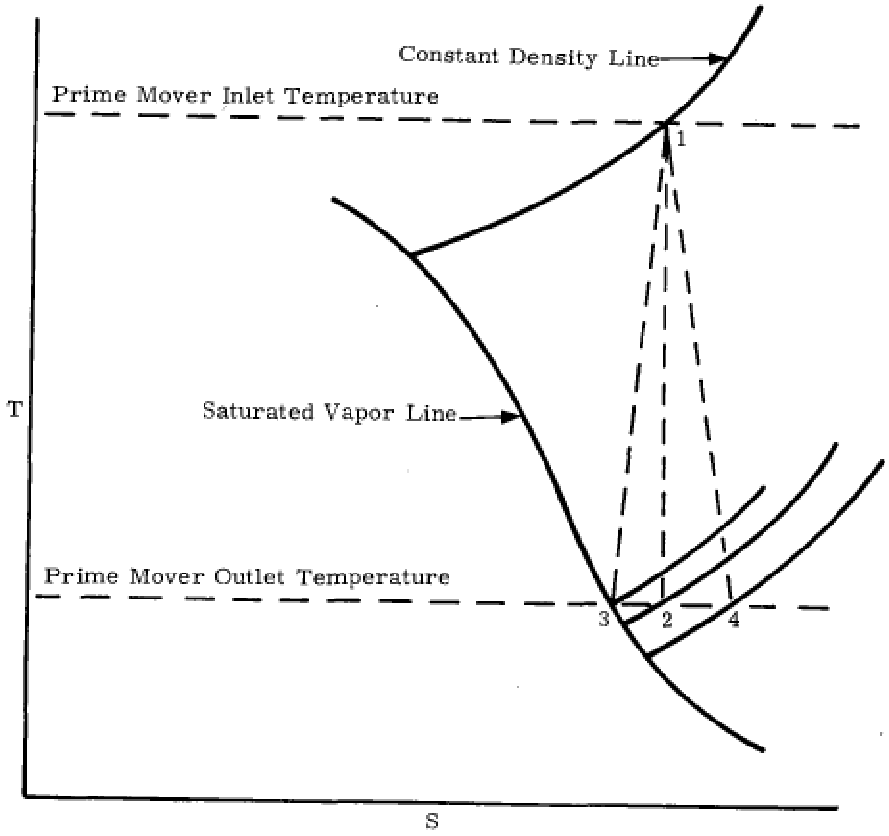


Figure 6-3. T-s diagram showing state points for error function calculations.

Beginning with the general relationship

$$u = f(T, v) \tag{6-26}$$

differentiating

$$du = \left(\frac{du}{dT}\right)_{\rho} dT + \left(\frac{du}{dv}\right)_{t} dv \quad . \tag{6-27}$$

Another thermodynamic equation, introduced in Section V, is

$$du = Tds - Pdv \tag{5-16}$$

dividing through by dv and holding temperature constant, we get

$$\left(\frac{du}{dv}\right)_{t} = T\left(\frac{ds}{dv}\right)_{t} - P \quad . \tag{6-28}$$

Substituting Eq. (5-13) into this equation yields

$$\left(\frac{du}{dv}\right)_t = T\left(\frac{dP}{dT}\right)_\rho - P \quad . \tag{6-29}$$

Now, substituting Eqs. (6-29) and (5-9) into (6-27) we get that

$$du = C_v dT + \left[T\left(\frac{dP}{dT}\right)_\rho - P\right] dv \tag{6-30}$$

substituting

$$v = 1/\rho \quad \text{and}$$

$$dv = -\frac{d\rho}{\rho^2} \quad \text{and}$$

rearranging we get that

$$du = C_v dT + \frac{T}{\rho^2}\left[\frac{P}{T} - \left(\frac{dP}{dT}\right)_\rho\right] d\rho \quad . \tag{6-31}$$

In integral form, this equation becomes

$$u_2 - u_1 = \int_{T_1}^{T_2} C_v dT + T \int_{\rho_1}^{\rho_2} \left[\frac{P}{T} - \left(\frac{dP}{dT}\right)_\rho\right] \frac{d\rho}{\rho^2} \tag{6-32}$$

where the ρ integral is evaluated at the initial temperature (T_1).

Substituting this equation in the equation

$$h_2 - h_1 = u_2 - u_1 + p_2 v_2 - p_1 v_1 \tag{6-33}$$

and transforming the equation into reduced variable form yields

$$h_2 - h_1 = \frac{P_c}{\rho_c}\left(\frac{p_2}{\phi_2} - \frac{p_1}{\phi_1}\right) + \int_{t_1}^{t_2} C_v T_c dt$$

$$+ Z_c R T_c t_1 \int_{\phi_1}^{\phi_2} \left[\frac{p}{t} - \left(\frac{dp}{dt}\right)_\rho\right] \frac{d\phi}{\phi^2} \quad . \tag{6-34}$$

This equation is good between any two points in the gaseous region.

The first term $\frac{P_c}{\rho_c}\left(\frac{p_2}{\phi_2} - \frac{p_1}{\phi_1}\right)$ is a straightforward calculation.

The second term is the integration of the constant volume specific heat, which has already been discussed somewhat. It is

$$\int_t C_v T_c dt = T_c \int_t \left[CP0 - FROJ + CP1 * T_c * t + CP2 * T_c^2 * t^2\right] dt \quad . \tag{6-35}$$

This integration yields

$$T_c \int_t C_v dt = T_c \left[(CP0 - FROJ)(t_2 - t_1) + \frac{CP1 * T_c}{2} * \left(t_2^2 - t_1^2\right) + \frac{CP2 * T_c^2}{3}\left(t_2^3 - t_1^3\right)\right] \quad . \tag{6-36}$$

The third term in Eq. (6-34) is the more difficult to evaluate. We must first generate the term shown within the brackets using the HBMS equation of state, then perform the integral.

The standard form of the HBMS equation is

$$\frac{p}{t} = -W_1(t) * \phi^2 - W_2(t) * \phi^3 + g(\phi) \quad . \tag{5-1}$$

It then follows that

$$p = -W_1(t) * t * \phi^2 - W_2(t) * t * \phi^3 + t * g(\phi) \tag{6-37}$$

and that

$$\left(\frac{dp}{dt}\right)_\rho = -\frac{d}{dt}\left(t * W_1(t)\right) * \phi^2 - \frac{d}{dt}\left(t * W_2(t)\right) * \phi^3 + g(\phi) \quad . \tag{6-38}$$

The bracketed term now becomes

$$\left[\frac{p}{t} - \left(\frac{dp}{dt}\right)_\rho\right] = -\left[W_1(t) - \frac{d}{dt}\left(t * W_1(t)\right)\right]\phi^2 - \left[W_2(t) - \frac{d}{dt}\left(t * W_2(t)\right)\right] * \phi^3 \tag{6-39}$$

and recalling that

$$W_1(t) = \frac{K_o}{t} + \frac{AW1}{t^2} \tag{6-40}$$

then

$$t * W_1(t) = K_o + \frac{AW1}{t} \tag{6-41}$$

and

$$\frac{d}{dt}\left(t * W_1(t)\right) = -\frac{AW1}{t^2} \tag{6-42}$$

and that

$$W_2(t) = AW2\left(1 - \frac{1}{t^2}\right) \tag{6-43}$$

then

$$t * W_2(t) = AW2\left(t - \frac{1}{t}\right) \tag{6-44}$$

and

$$\frac{d}{dt}\left(t * W_2(t)\right) = AW2\left(1 + \frac{1}{t^2}\right) . \tag{6-45}$$

Substituting Eqs. (6-40), (6-42), (6-43), and (6-45) into (6-39), the bracketed term now becomes

$$\left[\frac{p}{t} - \left(\frac{dp}{dt}\right)_\rho\right] = -\left[\frac{K_o}{t} + \frac{2AW1}{t^2}\right]\phi^2 - \left[\frac{AW2(t^2 - 1)}{t^2} - \frac{AW2(t^2 + 1)}{t^2}\right]\phi^3 \tag{6-46}$$

which can be reduced to

$$\left[\frac{p}{t} - \left(\frac{dp}{dt}\right)_\rho\right] = -\left[\frac{K_o}{t} + \frac{2AW1}{t^2}\right]\phi^2 + \frac{2 * AW2}{t^2}\,\phi^3 . \tag{6-47}$$

The integral now becomes

$$\int_{\phi}\left[\frac{p}{t}-\left(\frac{dp}{dt}\right)_{\rho}\right]\frac{d\phi}{\phi^{2}}=-\left[\frac{K_{o}}{t}+\frac{2AW1}{t^{2}}\right]\int_{\phi}d\phi+\frac{2*AW2}{t^{2}}\int_{\phi}\phi d\phi \quad . \qquad (6-48)$$

The integrated form is

$$\int_{\phi_1}^{\phi_2}\left[\frac{p}{t}-\left(\frac{dp}{dt}\right)_{\rho}\right]\frac{d\phi}{\phi^{2}}=-\left[\frac{K_{o}}{t}+\frac{2AW1}{t^{2}}\right]\left(\phi_{2}-\phi_{1}\right)+\frac{AW2}{t^{2}}\left(\phi_{2}^{2}-\phi_{1}^{2}\right) \quad . \qquad (6-49)$$

The final form of the equation for calculating the change in enthalpy between two state points is

$$\begin{aligned} h_{2}-h_{1} = {} & \frac{P_{c}}{\rho_{c}}\left[\frac{p_{2}}{\phi_{2}}-\frac{p_{1}}{\phi_{1}}\right]+T_{c}\left[(CP0-FROJ)(t_{2}-t_{1})\right. \\ & \left.+\frac{CP1*T_{c}}{2}\left(t_{2}^{2}-t_{1}^{2}\right)+\frac{CP2*T_{c}^{2}}{3}\left(t_{2}^{3}-t_{1}^{3}\right)\right] \\ & -Z_{c}*R*T_{c}*t_{1}\left\{\left[\frac{K_{o}}{t_{1}}+\frac{2AW1}{t_{1}^{2}}\right]\left(\phi_{2}-\phi_{1}\right)-\frac{AW2}{t_{1}^{2}}\left(\phi_{2}^{2}-\phi_{1}^{2}\right)\right\} \quad . \qquad (6-50) \end{aligned}$$

VII. Constant Pressure Heat Exchange in Gaseous Region

There are two processes where heat is either added to or taken from the working fluid while it exists as a gas at constant pressure. These two processes are superheating and regeneration which are used on several of the cycles either individually or together. The integrated equation, which will be generated in this section, is also used to calculate the state point after prime mover expansion. In this case, the heat generated due to the prime mover inefficiency, is put back into the fluid at constant pressure from the isentropic expansion state point. In this case, the heat added and the initial temperature are known, and a relatively simple iteration procedure is used to calculate the new temperature.

In this program, we are using a quadratic function of temperature to represent the constant pressure specific heat. The three constants in this equation are program inputs. The equation is

$$C_p = CP0 + CP1 * T + CP2 * T^2 \quad . \tag{7-1}$$

This equation is sometimes written in terms of reduced variables, and it then takes the form

$$C_p = CP0 + CP1 * T_c * t + CP2 * T_c^2 * t^2 \quad . \tag{7-2}$$

The change in enthalpy due to a constant pressure heat exchange is the integral of C_p with respect to temperature. The integral is

$$h_2 - h_1 = \int_T C_p dT \tag{7-3}$$

and the integrated form is

$$h_2 - h_1 = CP0 * (T_2 - T_1) + CP1 * \left(\frac{T_2^2 - T_1^2}{2}\right) + CP2 * \left(\frac{T_2^3 - T_1^3}{3}\right) . \tag{7-4}$$

VIII. Heat Rate for Boiling and Condensing

For all the subcritical cycles, the boiler vaporization heat rate and condenser heat rate are calculated with the same equation. The condenser heat rate for supercritical cycles also uses this equation. This equation is one of a number of general equations used to calculate the heat of vaporization and is referred to as the Chen Modification to the Pitzer Accentric Factor Correlation.[10] The accuracy of this equation is excellent. With 169 different fluids, the average error between the calculated and experimental values of the enthalpy of vaporization was 2.1 percent.[10]

The equation is

$$\Delta h = \frac{T(7.9\,t - 7.82 - 7.11\,\log_{10} P_{vp})}{(1.07 - t)(\text{Molecular Weight})} \quad . \qquad (8-1)$$

IX. Pump Work Calculations

The pump work for the cycle is calculated from the integral

$$W_P = \dot{m} \int_P v_l dP \tag{9-1}$$

where the limits on pressure are the condenser and boiler pressures. The specific volume of the liquid is considered constant, so this integral is reduced to the form

$$W_P = \dot{m} v_l (P_{Boiler} - P_{Condenser}) \quad . \tag{9-2}$$

The specific volume of the liquid was calculated at the condenser temperature by a combination of Mathia's method[10] and Benson's method.[10]

Mathia's method is an empirical equation relating a fluid's liquid density plus vapor density to the liquid density at the normal boiling temperature and the temperature where the density is to be calculated. The equation is

$$\rho_l + \rho_g = \rho_{lb} \frac{(2 - t)}{(2 - t_b)} \quad . \tag{9-3}$$

Benson's method is an empirical equation that relates the liquid density at the normal boiling point to the critical density and pressure. The equation is

$$\rho_{lb}/\rho_c = 0.422 \log_{10} P_c + 1.981 \quad . \tag{9-4}$$

In Mathia's method, the vapor density was neglected because it is small compared to the liquid density. Combining the two equations, we arrive at the following equation for calculating the specific volume of a liquid.

$$v_l = \frac{(2T_c - T_b)}{\rho_c (0.422 \log_{10} P_c + 1.981)(2T_c - T)} \quad . \tag{9-5}$$

Benson's method has been found to be accurate to within 3 percent for most organic and some inorganic liquids. Mathia's method has also been checked out extensively. Except in the vicinity of the critical point, this equation yields errors of only a few percent. Thus, the equation which results from combining these two equations appears to be sufficiently accurate for engineering purposes.

X. Boiler Liquid Heat Addition

For all subcritical cycles, the boiler heat addition is calculated by summing several individual heat rate calculations. These individual calculations are: 1) heat added to the liquid, 2) heat added for vaporization, and 3) heat added for superheating when appropriate. This section describes the calculation for the liquid heat addition.

The liquid heat addition is at constant pressure, just after the pump work. The calculation is made by integrating the constant pressure liquid heat capacity over the range of boiler temperature to condenser temperature. The liquid heat capacity is modeled by the equation

$$C_{pl} = CPL0 + CPL1 * T + CPL2 * T^2 \tag{10-1}$$

where CPL0, CPL1 and CPL2 are constants for each particular fluid and are inputed at program execution.

The variable name for the change in enthalpy due to the boiler liquid heat addition is DHBLH and is calculated with the following equation

$$DHBLH = \int_T C_{pl} dT \quad . \tag{10-2}$$

The integrated form is the only way it appears in the program and is

$$DHBLH = CPL0 * (T2 - T1) + CPL1 * (T2^2 - T1^2)/2$$

$$+ CPL2 * (T2^3 - T1^3)/3 \quad . \tag{10-3}$$

XI. Calculation of Nozzle Throat and Exit Areas

For a single stage impulse turbine, the entire pressure, temperature and enthalpy drop between points 1 and 2s in Figure 2-1 occurs in the nozzles. Under most cases of interest, the nozzles are of the supersonic variety with a minimum area section (throat) occurring between inlet and outlet of the nozzle. A typical converging-diverging supersonic nozzle is shown in Figure 11-1. At the throat, the area is a minimum as stated above, the product of vapor velocity and density is a maximum and the vapor velocity is the sonic velocity for the temperature and pressure existing in the throat (Mach number = 1).[11] The nozzle calculations in the program are based on the following.

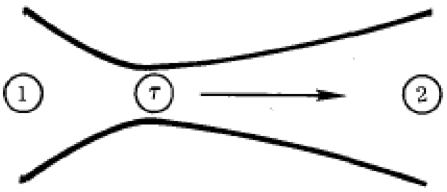


Figure 11-1. Typical supersonic nozzle cross-section. The arrow indicates the direction of mass flow and the circled quantities refer to state points in the derivation of the nozzle equations.

Conservation of Mass

$$\dot{m}_1 = \dot{m}_\tau = \dot{m}_2 \tag{11-1}$$

or equivalently

$$\rho_1 c_1 A_1 = \rho_\tau c_\tau A_\tau = \rho_2 c_2 A_2 \quad . \tag{11-2}$$

Conservation of Energy - Assume no heat losses or work into or out of the nozzle then

$$h_1 + \frac{c_1^2}{2gJ} = h_\tau + \frac{c_\tau^2}{2gJ} = h_2 + \frac{c_2^2}{2gJ} \quad . \tag{11-3}$$

Isentropic Process - Assume an ideal (frictionless, reversible) process then

$$s_1 = s_\tau = s_2 \quad . \tag{11-4}$$

Sonic Velocity at the Throat - From Reference 12

$$c_\tau^2 = \left(\frac{dP_\tau}{d\rho_\tau}\right)_s \quad . \tag{11-5}$$

From Eqs. (11-3) and (11-4) we can write

$$c_2^2 - c_1^2 = 2gJ(h_1 - h_{2s}) \quad . \tag{11-6}$$

From Eq. (11-2)

$$c_1 = \frac{\rho_2 c_2 A_2}{\rho_1 A_1} \quad . \tag{11-7}$$

Substituting Eq. (11-7) into (11-6) and manipulating we get

$$c_2^2 = \frac{2gJ(h_1 - h_{2s})}{\left[1 - \left(\frac{\rho_2 A_2}{\rho_1 A_1}\right)^2\right]} \quad . \tag{11-8}$$

Combining Eq. (11-8) with (11-1) and (11-2) and assuming a value for A_2/A_1 (this value is arbitrarily set at 1 in the program) we can solve for the nozzle exit area

$$A_2 = \frac{\dot{m}}{\rho_2 c_2} \quad . \tag{11-9}$$

$\dot{m}$, ρ_2, ρ_1 and $(h_1 - h_{2s})$ have already been calculated in the program.

At the throat we can write from Eq. (11-3)

$$h_1 - h_\tau = \frac{c_\tau^2 - c_1^2}{2gJ} \quad . \tag{11-10}$$

Substituting for c_1 from Eq. (11-7) into (11-10),

$$h_1 - h_\tau = \frac{c_\tau^2 - \left(\frac{\rho_2 A_2}{\rho_1 A_1}\right)^2 c_2^2}{2gJ} \quad . \tag{11-11}$$

Substituting for c_2 from Eq. (11-8) into (11-11) and manipulating

$$h_1 - h_\tau = \frac{c_\tau^2}{2gJ} + \frac{(h_1 - h_{2s})}{\left[\left(\frac{\rho_1 A_1}{\rho_2 A_2}\right)^2 - 1\right]} \quad . \tag{11-12}$$

To calculate the nozzle throat area, we must find c_τ and ρ_τ which then allows us to use Eqs. (11-1) and (11-2) to find A_τ similar to the procedure used in finding A_2. We note that c_τ is a function of ρ_τ (or P_τ) and T_τ as is $(h_1 - h_\tau)$ and s_τ. The method of solution in CYCLE is to make an initial estimate of ρ_τ and T_τ using perfect gas assumptions and then iterating to find a ρ_τ T_τ which satisfies Eqs. (11-4) and (11-12) simultaneously. The isentropic process derivation used to satisfy Eq. (11-4) is given in Section VI. and the enthalpy drop calculation for $(h_1 - h_\tau)$ is similar to that for the turbine enthalpy drop calculation described in Section VI. c_τ is not calculated from Eq. (11-5) directly since $(dP/d\rho)_s$ is not readily calculated explicitly using the HBMS equations and instead the following is used.

Writing the total derivative of $P(\rho, T)$

$$dP = \left(\frac{dP}{d\rho}\right)_t d\rho + \left(\frac{dP}{dT}\right)_\rho dT \quad . \tag{11-13}$$

Dividing through by $d\rho$ and specifying a constant entropy process

$$\left(\frac{dP}{d\rho}\right)_s = \left(\frac{dP}{d\rho}\right)_t + \left(\frac{dP}{dT}\right)_\rho \left(\frac{dT}{d\rho}\right)_s \quad . \tag{11-14}$$

Explicit equations for $\left(\frac{dP}{d\rho}\right)_t$ and $\left(\frac{dP}{dT}\right)_\rho$ are available in reduced form from HBMS and are given by Eqs. (5-26) and (5-27). To get $\left(\frac{dT}{d\rho}\right)_s$ in a form which can be explicitly calculated by the HBMS equations we proceed as follows

$$\left(\frac{dT}{d\rho}\right)_s = \left[\frac{dT}{d(1/v)}\right]_s = -v^2\left(\frac{dT}{dv}\right)_s \quad . \tag{11-15}$$

From the Bridgman tables[13]

$$\left(\frac{dT}{dv}\right)_s = \frac{(dv/dT)_p}{-\frac{1}{T}\left[C_p(dv/dP)_t + T(dv/dT)_p^2\right]} = \frac{T}{C_p(dv/dP)_t(dT/dv)_p + T(dv/dT)_p} \quad . \tag{11-16}$$

Writing the total derivative of P(v, T)

$$dP = \left(\frac{dP}{dv}\right)_t dv + \left(\frac{dP}{dT}\right)_v dT \quad . \tag{11-17}$$

For a constant pressure process, dP = 0 in Eq. (11-17) and

$$\left(\frac{dv}{dT}\right)_p = -\left(\frac{dP}{dT}\right)_v\left(\frac{dv}{dP}\right)_t \quad . \tag{11-18}$$

Substituting Eq. (11-18) into (11-16) we get

$$\left(\frac{dT}{dv}\right)_s = \frac{-T}{C_p\left(\frac{dT}{dP}\right)_v + T\left(\frac{dv}{dP}\right)_t\left(\frac{dP}{dT}\right)_v} \tag{11-19}$$

Writing Eq. (11-19) in terms of ρ we get

$$-\rho^2\left(\frac{dT}{d\rho}\right)_s = \frac{-T}{C_p\left(\frac{dT}{dP}\right)_\rho - \frac{T}{\rho^2}\left(\frac{d\rho}{dP}\right)_t\left(\frac{dP}{dT}\right)_\rho} \tag{11-20}$$

or

$$\left(\frac{dT}{d\rho}\right)_s = \frac{T}{\rho^2 C_p\left(\frac{dT}{dP}\right)_\rho - T\left(\frac{d\rho}{dP}\right)_t\left(\frac{dP}{dT}\right)_\rho} \quad . \tag{11-21}$$

Substituting Eq. (11-21) into (11-14) we get

$$\left(\frac{dP}{d\rho}\right)_s = \frac{\left(\frac{dP}{d\rho}\right)_t^2}{\left(\frac{dP}{d\rho}\right)_t - \frac{T}{\rho^2 C_p}\left(\frac{dP}{dT}\right)_\rho^2} \quad . \tag{11-22}$$

Alternately, we can substitute for $T\left(\frac{dP}{dT}\right)_\rho^2$ from Eq. (5-24) into (11-22) to get

$$\left(\frac{dP}{d\rho}\right)_s = \frac{C_p}{C_v}\left(\frac{dP}{d\rho}\right)_t \tag{11-23}$$

or we could solve for C_p from Eq. (5-32) and substitute into Eq. (11-22) to get

$$\left(\frac{dP}{d\rho}\right)_s = \left(\frac{dP}{d\rho}\right)_t + \frac{T}{C_v\rho^2}\left(\frac{dP}{dT}\right)_\rho^2 \quad . \tag{11-24}$$

Although Eq. (11-23) appears to be the simplest, Eqs. (11-22), (11-23), and (11-24) require the same computation time and Eq. (11-24) is the form for c_τ^2 which actually appears in the program.

APPENDIX A

The use of Program CYCLE is best illustrated by examples. The form of the program presented in this report is the timesharing version presently operational on Sandia's CDC 6600 NOS system. The examples presented at the end of this appendix illustrate the five basic cycles shown in Figure 3-1. The input required by the user is underlined in the examples.

It should be noted that the efficiencies and total input heat rates are given in each case for the regenerative and the nonregenerative case, but all other program output assumes regeneration is present. If a nonregenerative cycle is to be considered in detail, the regenerator efficienty should be entered as zero. Similarly, various other cycle configurations can be simulated by choosing appropriate values for the various efficiencies. For example, if the prime mover does not drive a generator and only shaft work is required, the equivalent work output in kW should be entered and the generator efficiency should be entered as one.

Example Program Executions:

```
$ATLIB(CSLIB)
/lgo.
  WORKING FLUID IS? toluene
  GENERATOR EFFICIENCY IS ? .9
  TURBINE EFFICIENCY =? .65
  REGENERATOR EFFICIENCY =? .8
  NOZZLE EFFICIENCY = ? .95
  PUMP EFFICIENCY = ? .3
  ELECTRICAL POWER OUTPUT (KW) =? 100
  LOW TEMP. (DEG F) = ? 165
  HIGH TEMP. (DEG F) =? 550
  WANT TO ENTER HIGH PRESSURE ? no

  SUB-CRITICAL DRYING FLUID CYCLE
  BOILER TEMP = 550.0 DEGREES F          BOILER PRESSURE = 409.57 PSIA
  COND TEMP = 165.00 DEGREES F    COND PRESSURE =   4.82 PSIA
  NOZZLE EXIT TEMP(ISENTROPIC) =305.575 DEGREES F
  TURBINE EXHAUST TEMP = 372.69 DEGREES F
  NOZZLE SPOUTING VEL =1853.65  FT/SEC
  NOZZLE EXIT MACH NUMBER(ISENTROPIC) =2.968
  NOZZLE THROAT AREA = .171393     SQUARE INCHES
  NOZZLE EXIT AREA = 3.37266     SQUARE INCHES
  BOILER FEED PUMP = 16.435     HP
  MASS FLOW RATE = 8514.68     LBM/HR
  PUMP VOLUMETRIC FLOW = 20.946     GAL/MIN
  TURBINE EXHAUST FLOW = 2592.29     CUBIC FT/MIN
  TURBINE ISENTROPIC HEAD = 76.083     BTU/LBM
  TURBINE SPECIFIC SPEED ( ROTOR DIA.= 1 FT.) = 30.67
  TURBINE SPECIFIC DIAMETER ( ROTOR DIA.=1 FT.) = 2.373
  BOILER HEAT RATE (NO REGENERATION) = 2424016.6     BTU/HR
     OF WHICH  1791129.3     BTU/HR IS HEAT ADDED TO LIQUID
               632887.33     BTU/HR IS FOR VAPORIZATION
               0.            BTU/HR IS FOR SUPERHEATING
  BOILER HEAT RATE (WITH REGENERATION) = 1908255.9     BTU/HR
  CONDENSER HEAT RATE(WITH REGENERATION) = 1525829.5     BTU/HR
  REGENERATOR HEAT RATE(VAPOR SIDE)= 644700.86     BTU/HR
  REGENERATOR HEAT RATE(LIQUID SIDE) = 515760.69     BTU/HR
  TEMP OF LIQUID OUTPUT FROM REGENERATOR =  302.54     DEGREES F
  SUPERHEATER HEAT RATE =  0.              BTU/HR
  EFFICIENCY (WITHOUT REG)= 14.1 %
  EFFICIENCY (WITH REG)= 17.9 %
  CARNOT EFFICIENCY = 38.1 %


  ANY MORE TEMPERATURES ? yes
```

Examples (cont)

```
LOW TEMP. (DEG F) = ? 165
HIGH TEMP. (DEG F) =? 550
WANT TO ENTER HIGH PRESSURE ? yes
ENTER HIGH PRESSURE(PSIA) LESS THAN 409.56
HIGH PRESSURE (PSIA) =? 230

SUB-CRITICAL DRYING FLUID CYCLE WITH SUPERHEAT AND REGERERATION
SUPERHEAT TEMP = 550.0 DEGREES F  SUPERHEAT PRESSURE = 230.00 PSIA
NOZZLE EXIT TEMP(ISENTROPIC) =359.578 DEGREES F
TURBINE EXHAUST TEMP = 419.95 DEGREES F
COND TEMP = 165.00 DEGREES F    COND PRESSURE =   4.82 PSIA
BOILER TEMP = 475.2 DEGREES F         BOILER PRESSURE = 230.00 PSIA
NOZZLE SPOUTING VEL =1805.47  FT/SEC
NOZZLE EXIT MACH NUMBER(ISENTROPIC) =2.796
NOZZLE THROAT AREA = .377390     SQUARE INCHES
NOZZLE EXIT AREA = 3.74171     SQUARE INCHES
BOILER FEED PUMP = 9.2174     HP
MASS FLOW RATE = 8583.25     LBM/HR
PUMP VOLUMETRIC FLOW = 21.114     GAL/MIN
TURBINE EXHAUST FLOW = 2827.00     CUBIC FT/MIN
TURBINE ISENTROPIC HEAD = 72.180     BTU/LBM
TURBINE SPECIFIC SPEED ( ROTOR DIA.= 1 FT.) = 32.45
TURBINE SPECIFIC DIAMETER ( ROTOR DIA.=1 FT.) = 2.242
BOILER HEAT RATE (NO REGENERATION) = 2611800.6     BTU/HR
   OF WHICH  1380846.6     BTU/HR IS HEAT ADDED TO LIQUID
             930927.29     BTU/HR IS FOR VAPORIZATION
             300026.65     BTU/HR IS FOR SUPERHEATING
BOILER HEAT RATE (WITH REGENERATION) = 1955199.1     BTU/HR
CONDENSER HEAT RATE(WITH REGENERATION) = 1572289.3     BTU/HR
REGENERATOR HEAT RATE(VAPOR SIDE)= 820751.89     BTU/HR
REGENERATOR HEAT RATE(LIQUID SIDE) = 656601.51     BTU/HR
TEMP OF LIQUID OUTPUT FROM REGENERATOR =  330.29     DEGREES F
SUPERHEATER HEAT RATE =  300026.65     BTU/HR
EFFICIENCY (WITHOUT REG)= 13.1 %
EFFICIENCY (WITH REG)= 17.5 %
CARNOT EFFICIENCY = 38.1 %


ANY MORE TEMPERATURES ? yes
```

Examples (cont)

```
LOW TEMP. (DEG F) = ? 190
HIGH TEMP. (DEG F) =? 825
HIGH TEMP. ENTERED IS ABOVE OPERATING TEMP.
HIGH PRESSURE (PSIA) =? 800

SUPERCRITICAL DRYING FLUID CYCLE
SUPERHEAT TEMP = 825.0 DEGREES F  SUPERHEAT PRESSURE = 800.00 PSIA
NOZZLE EXIT TEMP(ISENTROPIC) =563.442 DEGREES F
TURBINE EXHAUST TEMP = 638.65 DEGREES F
COND TEMP = 190.00 DEGREES F    COND PRESSURE =   7.55 PSIA
NOZZLE SPOUTING VEL =2199.83  FT/SEC
NOZZLE EXIT MACH NUMBER(ISENTROPIC) =3.059
NOZZLE THROAT AREA = .315359E-01 SQUARE INCHES
NOZZLE EXIT AREA = 1.81008      SQUARE INCHES
BOILER FEED PUMP = 24.345      HP
MASS FLOW RATE = 6334.90     LBM/HR
PUMP VOLUMETRIC FLOW = 15.847      GAL/MIN
TURBINE EXHAUST FLOW = 1670.19      CUBIC FT/MIN
TURBINE ISENTROPIC HEAD = 107.16      BTU/LBM
TURBINE SPECIFIC SPEED ( ROTOR DIA.= 1 FT.) = 22.60
TURBINE SPECIFIC DIAMETER ( ROTOR DIA.=1 FT.) = 3.220
BOILER HEAT RATE (NO REGENERATION) = 2608336.1      BTU/HR
BOILER HEAT RATE (WITH REGENERATION) = 1640649.0      BTU/HR
CONDENSER HEAT RATE(WITH REGENERATION) = 1261426.7      BTU/HR
REGENERATOR HEAT RATE(VAPOR SIDE)= 1209608.9      BTU/HR
REGENERATOR HEAT RATE(LIQUID SIDE) = 967687.09      BTU/HR
TEMP OF LIQUID OUTPUT FROM REGENERATOR =  485.53      DEGREES F
SUPERHEATER HEAT RATE =  0.               BTU/HR
EFFICIENCY (WITHOUT REG)= 13.1 %
EFFICIENCY (WITH REG)= 20.8 %
CARNOT EFFICIENCY = 49.4 %


ANY MORE TEMPERATURES ? no
    .358 CP SECONDS EXECUTION TIME
```

Examples (cont)

```
1go.
 WORKING FLUID IS? water
 GENERATOR EFFICIENCY IS ? .9
 TURBINE EFFICIENCY =? .65
 REGENERATOR EFFICIENCY =? .8
 NOZZLE EFFICIENCY = ? .95
 PUMP EFFICIENCY = ? .3
 ELECTRICAL POWER OUTPUT (KW) =? 100
 LOW TEMP. (DEG F) = ? 165.
 HIGH TEMP. (DEG F) =? 550.
 WANT TO ENTER HIGH PRESSURE ? no

 SUB-CRITICAL WETTING FLUID CYCLE
 BOILER TEMP = 270.3 DEGREES F          BOILER PRESSURE =  40.55 PSIA
 SUPERHEAT TEMPERATURE =    550.00 DEGREES F
 NOZZLE EXIT TEMP(ISENTROPIC) =165.000 DEGREES F
 TURBINE EXHAUST TEMP = 300.30 DEGREES F
 NOZZLE EXIT TEMP(ISENTROPIC) =165.000 DEGREES F
 COND TEMP = 165.00 DEGREES F    COND PRESSURE =   5.65 PSIA
 NOZZLE SPOUTING VEL =2805.99  FT/SEC
 NOZZLE EXIT MACH NUMBER(ISENTROPIC) =1.956
 NOZZLE THROAT AREA = 1.73481     SQUARE INCHES
 NOZZLE EXIT AREA = 3.14128     SQUARE INCHES
 BOILER FEED PUMP = .46772     HP
 MASS FLOW RATE = 3356.89     LBM/HR
 PUMP VOLUMETRIC FLOW = 6.9118     GAL/MIN
 TURBINE EXHAUST FLOW = 3672.66     CUBIC FT/MIN
 TURBINE ISENTROPIC HEAD = 174.34     BTU/LBM
 TURBINE SPECIFIC SPEED ( ROTOR DIA.= 1 FT.) = 29.67
 TURBINE SPECIFIC DIAMETER ( ROTOR DIA.=1 FT.) = 2.453
 BOILER HEAT RATE (NO REGENERATION) = 4043313.7     BTU/HR
    OF WHICH  348008.15     BTU/HR IS HEAT ADDED TO LIQUID
              3260770.6     BTU/HR IS FOR VAPORIZATION
              434534.94     BTU/HR IS FOR SUPERHEATING
 BOILER HEAT RATE (WITH REGENERATION) = 3879443.3     BTU/HR
 CONDENSER HEAT RATE(WITH REGENERATION) = 3532015.6     BTU/HR
 REGENERATOR HEAT RATE(VAPOR SIDE)= 204838.07     BTU/HR
 REGENERATOR HEAT RATE(LIQUID SIDE) = 163870.46     BTU/HR
 TEMP OF LIQUID OUTPUT FROM REGENERATOR =  214.74     DEGREES F
 SUPERHEATER HEAT RATE =  434534.94     BTU/HR
 EFFICIENCY (WITHOUT REG)=  8.4 %
 EFFICIENCY (WITH REG)=  8.8 %
 CARNOT EFFICIENCY = 38.1 %


 ANY MORE TEMPERATURES ? yes
```

Examples (cont)

```
LOW TEMP. (DEG F) = ? 220
HIGH TEMP. (DEG F) =? 1910
WANT TO ENTER HIGH PRESSURE ? no

SUPERCRITICAL WETTING FLUID CYCLE
 SUPERHEAT TEMP =1910.0 DEGREES F  SUPERHEAT PRESSURE =3259.54 PSIA
 NOZZLE EXIT TEMP(ISENTROPIC) =275.373 DEGREES F
 TURBINE EXHAUST TEMP = 880.89 DEGREES F
 COND TEMP = 220.00 DEGREES F     COND PRESSURE =  17.07 PSIA
 NOZZLE SPOUTING VEL =6101.85  FT/SEC
 NOZZLE EXIT MACH NUMBER(ISENTROPIC) =3.934
 NOZZLE THROAT AREA = .796226E-02 SQUARE INCHES
 NOZZLE EXIT AREA = .126136     SQUARE INCHES
 BOILER FEED PUMP = 10.107      HP
 MASS FLOW RATE = 755.695     LBM/HR
 PUMP VOLUMETRIC FLOW = 1.6078      GAL/MIN
 TURBINE EXHAUST FLOW = 319.047     CUBIC FT/MIN
 TURBINE ISENTROPIC HEAD = 824.44      BTU/LBM
 TURBINE SPECIFIC SPEED ( ROTOR DIA.= 1 FT.) = 5.930
 TURBINE SPECIFIC DIAMETER ( ROTOR DIA.=1 FT.) = 12.27
 BOILER HEAT RATE (NO REGENERATION) = 1375780.1      BTU/HR
 BOILER HEAT RATE (WITH REGENERATION) = 1186207.3      BTU/HR
 CONDENSER HEAT RATE(WITH REGENERATION) = 806985.04      BTU/HR
 REGENERATOR HEAT RATE(VAPOR SIDE)= 236966.11      BTU/HR
 REGENERATOR HEAT RATE(LIQUID SIDE) = 189572.89      BTU/HR
 TEMP OF LIQUID OUTPUT FROM REGENERATOR =  479.43      DEGREES F
 SUPERHEATER HEAT RATE =  0.            BTU/HR
 EFFICIENCY (WITHOUT REG)= 24.8 %
 EFFICIENCY (WITH REG)= 28.8 %
 CARNOT EFFICIENCY = 71.3 %


ANY MORE TEMPERATURES ? no
     .540 CP SECONDS EXECUTION TIME
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```
      PROGRAM CYCLE(INPUT=201,OUTPUT=201,TAPE1=INPUT,TAPE2=OUTPUT,TAPE3)
C  BY J.P. ABBIN AND W.R.LEUENBERGER
C     CONVERTED TO NOS BY C.B. ROGERS APR 77
C    LAST REVISED JULY 22, 77 PUT IN TECH MEMO CORR TO PH3,COPH1
      COMMON AR1,AR2,AR3,AR4,RHCR,R
      COMMON AKO,AW1,AW2,ZC,AJ,AGC
      COMMON TOPR,POPR
      COMMON /FLUID/ BETA,ALPHC,CP0,CP1,CP2,TCR,PCR,TBL,GPGM
     1 ,CPL0,CPL1,CPL2
      COMMON /TYFIN/ NAME,ETGN,ETT,ETR,ETN,ETP,EPR,TLOW,THIGH
      PH1(RR)=ATAN((2.*AR4*RR-AR3)/(4.*AR2*AR4-AR3**2)**(.5))
      PH2(RHR)=ALOG(RHR**2/(AR2-AR3*RHR+AR4*RHR**2))
      BT1(T)=AJ*((CP0-FROJ)*ALOG(T*TCR)+CP1*T*TCR+CP2*(T*TCR)**2/2.)/R
      G(RHR)=AR1*RHR/(AR2-AR3*RHR+AR4*RHR**2)
      W1(TR)=AKO/TR+AW1/TR**2
      W2(TR)=AW2*(1.-1./TR**2)
      PKCF(T)=14.7*(PCR/14.7)**((1.-TBL/T)/(1.-TBL/TCR))
      PH3(RHR,TR)=AW1*RHR/TR**2-AW2*(TR**2+1.)*RHR**2/(2.*TR**2)
      DHCM(TR,PR)=(7.9*TR-7.82-7.11*ALOG10(PR))/(1.07-TR)
      FTR(T1,T2,R1,R2)=(BT1(T1)-BT1(T2))/ZC+COPH2*(PH2(R2)-PH2(R1))+COPH
     11*(PH1(R2)-PH1(R1))+PH3(R2,T1)-PH3(R1,T1)
      PCHECK(T)=-AKO-AW1/T-AW2*(T**2-1.)/T+AR1*T/(AR2-AR3+AR4)
      DPDRH(TR,RHR)=-2.*(AKO+AW1/TR)*RHR-3.*AW2*(RHR**2)*(TR**2-1.)
     1/TR+TR*AR1*(AR2-AR4*RHR**2)/(AR2-AR3*RHR+AR4*RHR**2)**2
      DPDT(TR,RHR)=(AW1*RHR**2)/TR**2-AW2*RHR**3*(TR**2+1.)
     1/TR**2+AR1*RHR/(AR2-AR3*RHR+AR4*RHR**2)
      CV(TR,RHR)=CP0+CP1*(TR*TCR)+CP2*(TR*TCR)**2-ZC*R*TR*(DPDT
     1(TR,RHR))**2/(AJ*(DPDRH(TR,RHR))*RHR**2)
      C2(TR,RHR)=ZC*AGC*R*TCR*(DPDRH(TR,RHR)+ZC*TR*R*((DPDT(TR,RHR)
     1)**2)/(AJ*(RHR**2)*CV(TR,RHR)))
      DHHO(TR,RHR)=-ZC*(R/AJ)*TR*TCR*(RHR*(2.*AKO/TR+3.*AW1/TR**2)
     1+(AW2*RHR**2)*(1.-2./TR**2))+(R/AJ)*TR*TCR*(AR3*RHR-
     2AR4*RHR**2)/(AR2-AR3*RHR+AR4*RHR**2)+
     3CP0*TR*TCR+(CP1*(TR*TCR)**2)/2.+(CP2*(TR*TCR)**3)/3.

   10 PRINT*,≠ WORKING FLUID IS≠,
      READ (1,48) NAME
        IF(EOF(1)) 10,12
C  11 NAME=3HWAT
C  NOW GET FLUID PARAMETERS
   12 IERR= 10
      CALLGETF(IERR,3,NAME,7LJPABBIN)
      IF(IERR .EQ. 0) GO TO 13
      PRINT*,≠ PROBLEM WITH FLUID FILE, IERR=≠,IERR
       GO TO 10
   13 READ(3,*) BETA,ALPHC,CP0,CP1,CP2,TCR,PCR,TBL,GPGM,CPL0,CPL1,CPL2
      IF(EOF(3)) 2040,14
 2040 PRINT*,≠ EOF FROM FLUID FILE≠
      STOP

   14 PRINT*,≠ GENERATOR EFFICIENCY IS≠,
      READ*, ETGN
      IF(EOF(1)) 14,16
C  15 ETGN= .9
   16 CONTINUE
      IF( ETGN.GE. 0. .AND.  ETGN .LE. 1.0) GO TO 18
      PRINT*,≠ ETGN OUT OF RANGE≠
```

```
         GO TO 14

      18 PRINT*,≠ TURBINE EFFICIENCY =≠,
         READ*, ETT
         IF(EOF(1)) 18,20
C     19 ETT = .65
      20 IF(ETT .GE. 0. .AND. ETT .LE. 1.0) GO TO 22
         PRINT*,≠ ETT OUT OF RANGE≠
         GO TO  18

      22 PRINT*,≠ REGENERATOR EFFICIENCY =≠,
         READ*, ETR
         IF(EOF(1)) 22,24
C     23 ETR = .8
      24 IF(ETR .GE. 0. .AND. ETR.LE. 1.) GO TO 26
         PRINT*,≠ ETR OUT OF RANGE≠
         GO TO 22

      26 PRINT*,≠ NOZZLE EFFICIENCY =≠,
         READ*, ETN
         IF(EOF(1)) 26,28
C     27 ETN = .95
      28 IF(ETN .GE. 0. .AND.ETN .LE. 1.) GO TO 30
         PRINT*,≠ ETN OUT OF RANGE≠
         GO TO 26

      30 PRINT*,≠ PUMP EFFICIENCY =≠,
         READ*, ETP
         IF(EOF(1)) 30,32
C     31 ETP = .3
      32 IF(ETP.GE. 0. .AND. ETP .LE. 1.) GO TO 34
         PRINT*,≠ ETP OUT OF RANGE≠
         GO TO 30

      34 PRINT*,≠ ELECTRICAL POWER OUTPUT (KW) =≠,
         READ*, EPR
         IF(EOF(1)) 34,36
C     35 EPR = 100.
      36 IF(EPR .GE. 0.) GO TO 38
         PRINT*,≠ EPR OUT OF RANGE≠
         GO TO 34

      38 AKO=4.71
         AW1=BETA-AKO
         AW2=(1.-AKO-ALPHC+2.*BETA)/2.
         AR1=(1.+BETA)**3
         AR2=BETA*(3.*BETA-1.)
         AR3=3.*BETA**2-6.*BETA-1.
         AR4=BETA*(BETA-3.)
         ZC=BETA*(3.*BETA-1.)/(1.+BETA)**3
         COPH1=( +AR3/(4.*AR2*AR4-AR3**2)**(.5) )*AR1/AR2
         COPH2=AR1/(2.*AR2)
         R=1545./GPCM
         RHCR=PCR*144./(ZC*R*TCR)
         AJ=777.649
         AGC=32.174
         A1A2=1.
```

```
            TKCR=5.*TCR/9.
            TKB=5.*TBL/9.
            NO=0
            NOS=0
            TOPR=.95*TCR
            POPR=PKCF(TOPR)

      40    PRINT*,≠ LOW TEMP. (DEG F) =≠,
            READ*, TLOW
            IF(EOF(1))40,42
C     41    TLOW = 165.
      42    TLOW=TLOW+459.69
      43    PRINT*,≠ HIGH TEMP. (DEG F) =≠,
            READ*, THIGH
            IF(EOF(1)) 43,44
C     43    THIGH = 550.
C     44    PRINT 45, NAME,ETGN, ETT, ETR, ETN, ETP, EPR
      45    FORMAT(*0 FLUID  GEN EF  TUR EF  REG EF  NOZ EF  PMP EF*
          1 ,*   PWR (KW)*,/, 2X,A3, 1X, 5(F8.3), F10.1, / )
      44    TLOWP= TLOW - 459.69
            THIGH=THIGH+459.69
            T3=TLOW
            IF (TLOW.GE.THIGH) GO TO 450
            TKC=5.*TLOW/9.
            TKL=5.*TLOW/9.
            TKH=5.*THIGH/9.
            T1P=THIGH
            IF (THIGH.GE.TOPR) GO TO 46
            THAVE=THIGH
            GO TO 47
      46    THAVE=TCR
      47    TAVE=(THAVE+TLOW)/2.
            TKAVE=TAVE*5./9.
            TR=TAVE/TCR
            PAVE=PKCF(TAVE)
            PR=PAVE/PCR
            CPV=CP0+CP1*TAVE+CP2*TAVE**2
            DHV=454.*TKAVE*DHCM(TR,PR)/(252.*GPGM)
            DSDT=(CPV-CHV/TAVE)/TAVE
            SDSDT=DSDT/ABS(DSDT)
            IF (THIGH.GE.TOPR) GO TO 66
            IF (SDSDT.GE.0.0) GO TO 54
            PRINT*,≠ WANT TO ENTER HIGH PRESSURE ≠,
             READ(1,48) IQB
      48    FORMAT(A3)
            IF(EOF(1)) 51,52
      51    IQB = 2HNO

      52    NO=3
            IF(IQB .EQ. 3HYES) GO TO 110
            NO=4
            GO TO 280
      54    PCALC=PKCF(THIGH)
            PRINT*,≠ WANT TO ENTER HIGH PRESSURE ≠,
            READ(1,48) IQC
            IF(EOF(1)) 170,56
      56    CONTINUE
```

```
      IF(IQC .EQ.  3HYES ) GO TO 58
      GO TO 170
   58 PRINT*,≠ ENTER HIGH PRESSURE(PSIA) LESS THAN ≠, PCALC
      PHIGH = PCALC
      PRINT*,≠ HIGH PRESSURE (PSIA) =≠,
      READ*, PHIGH
      IF(EOF(1)) 58,70
 66    IF (SDSOT.LE.0.0) GO TO 110
      PRINT*,≠ HIGH TEMP. ENTERED IS ABOVE OPERATING TEMP.≠
      PRINT*,≠ HIGH FRESSURE (PSIA) =≠,
      PHIGH = PCR
      READ*, PHIGH
      IF(EOF(1)) 80,67
   67 CONTINUE
      IF (PHIGH.GE.PCR) GO TO 80
   70 PRINT 72
   72 FORMAT( /,*  SUB-CRITICAL DRYING FLUID CYCLE*
     1 ,* WITH SUPERHEAT AND REGERERATION* )
      NO=2
      GO TO 180
 80   CONTINUE
      PR=PHIGH/PCR
      TRH=THIGH/TCR
      W1T=W1(TRH)
      W2T=W2(TRH)
      IF (PR.GE.PCHECK(TRH)) GO TO 90
      RHHIGH=RHO(PR,TRH,W1T,W2T)
      RHRHI=RHHIGH/RHCR
      PLOW=PKCF(TLOW)
      TRL=TLOW/TCR
      PR=PLOW/PCR
      W1T=W1(TRL)
      W2T=W2(TRL)
      RHLOW=RHO(PR,TRL,W1T,W2T)
      RHRLOW=RHLOW/RHCR
      FTRCK=FTR(TRH,TRL,RHRHI,RHRLOW)
      IF (FTRCK.GE.0.0) GO TO 100
   90 PRINT*,≠ EXPANSION INTO QUALITY REGION≠
      GO TO 450
  100 PRINT*,1H
      PRINT*,≠ SUPERCRITICAL DRYING FLUID CYCLE≠
      NO=1
      GO TO 180
 110  CONTINUE
      NOS=1
      GO TO 280
 120  PCALC=P2
      IF (PCALC.GE.PCR) GO TO 130
      IF(NO.EQ.3) GO TO 140
      IF (NOS.EQ.1) GO TO 130
      PRINT*,≠ WANT TO ENTER HIGH PRESSURE≠,
      READ(1,48) IQD
      IF(EOF(1)) 320,128
  128 CONTINUE
      IF(IQD .EQ. 3HYES) GO TO 130
      GO TO 320
```

```
 130  CONTINUE
      PRINT*,≠ WANT TO ENTER HIGH PRESSURE≠,
      READ(1,48) IQB
      IF(EOF(1)) 138,139
  138 IQB = 2HNO
  139 CONTINUE
      IF(IQB .EQ. 3HYES) GO TO 140
      PHIGH=PCALC
      GO TO 142
  140 PRINT*,≠ ENTER HIGH PRESSURE(PSIA) LESS THAN≠, PCALC
      PRINT*,≠ HIGH PRESSURE (PSIA) =≠,
      PHIGH = PCALC
      READ*, PHIGH
      IF(EOF(1)) 140,142
 142  IF (PHIGH.GT.PCALC) GO TO 90
      IF (PHIGH.GE.PCR) GO TO 150
      PRINT 145
  145 FORMAT( /,* SUB-CRITICAL WETTING FLUID CYCLE*
    1 , * WITH SUPERHEAT AND REGENERATION* )
      GO TO 160
  150 PRINT 152
  152 FORMAT( /, * SUPERCRITICAL WETTING FLUID CYCLE* )
      NO = 1
      GO TO 180
 160  CONTINUE
      NO=2
      GO TO 180
 170  P1P=PKCF(THIGH)
      PHIGH=P1P
      P3=PKCF(TLOW)
      P2P=P3
      PLOW=P3
      GO TO 190
 180  P1P=PHIGH
      P3=PKCF(TLOW)
      P2P=P3
      PLOW=P3
 190  PR1P=P1P/PCR
      TR1P=THIGH/TCR
      P=PR1P
      T=TR1P
      W1T=W1(T)
      W2T=W2(T)
      IF (NO.EQ.0) GO TO 200
      IF (THIGH.LE.TCR) GO TO 200
      IF (P.GE.PCHECK(T)) GO TO 90
 200  RH1P=RHO(P,T,W1T,W2T)
      RHR1P=RH1P/RHCR
      T2P=(THIGH+TLOW)/2.
 210  TR2P=T2P/TCR
      FROJ=SFROJ(T1P,P1P,RH1P,T2P,P2P)
      P=PLOW/PCR
      W2T=W2(TR2P)
      W1T=W1(TR2P)
      RH2P1=RHO(P,TR2P,W1T,W2T)
 220  RH2P2=1.05*RH2P1
      RHR2P1=RH2P1/RHCR
```

```
      RHR2P2=RH2P2/RHCR
      FTR2=FTR(TR1P,TR2P,RHR1P,RHR2P2)
      FTR1=FTR(TR1P,TR2P,RHR1P,RHR2P1)
      RHR2P2=-(RHR2P2-RHR2P1)*FTR1/(FTR2-FTR1)+RHR2P1
      IF (RHR2P2.GE.0.0) GO TO 230
      RHR2P2=RHR2P1/2.
  230 CONTINUE
      IF (ABS(FTR(TR1P,TR2P,RHR1P,RHR2P2)).LE..00001) GO TO 240
      RH2P1=RHR2P2*RHCR
      GO TO 220
  240 P2P1=PCR*TR2P*(-W1(TR2P)*RHR2P2**2-W2(TR2P)*RHR2P2**3+G(RHR2P2))
      IF (ABS(P2P1-PLOW).LE..1) GO TO 250
      T2P=T2P*(P3/P2P1)**(.05)
      GO TO 210
  250 P2P=P2P1
      RH2P=RHR2P2*RHCR
      DHT=((P2P/RH2P)-(P1P/RH1P))*144./AJ+(CP0-FROJ)*(T2P-T1P)+CP1*(T2P*
     1*2-T1P**2)/2.+CP2*(T2P**3-T1P**3)/3.+ZC*R*T1P*(-((AKO/TR1P)+(2.*AW
     21/(TR1P**2)))*(RHR2P2-RHR1P)+(AW2*(RHR2P2**2-RHR1P**2)/TR1P**2))/A
     3J
      IF (NO.EQ.1) GO TO 260
      IF (NO.EQ.2) GO TO 260
      DHBLH=CPL0*(THIGH-TLOW)+CPL1*(THIGH**2-TLOW**2)/2.
     1+CPL2*(THIGH**3-TLOW**3)/3.
  260 CONTINUE
      DHR=CP0*(T3-T2P)+CP1*(T3**2-T2P**2)/2.+CP2*(T3**3-T2P**3)/3.
      DHR=-DHR-DHT*(1.-ETT)
      IF (NO.EQ.2) GO TO 270
      DHSH=0.0
      IF (NO.EQ.1) GO TO 350
      TR=THIGH/TCR
      PR=P1P/PCR
      GO TO 340
  270 P2=PHIGH
      T2=THIGH
      RH3P=RH2P
      GO TO 320
  280 T3P=TLOW
      T2=THIGH
      TR2=T2/TCR
      P3P=PKCF(TLOW)
      PLOW=P3P
      PR3P=P3P/PCR
      TR3P=T3P/TCR
      W1T=W1(TR3P)
      W2T=W2(TR3P)
      RH3P=RHO(PR3P,TR3P,W1T,W2T)
      RHR3P=RH3P/RHCR
      RHR21=RHR3P*(T2/T3P)**2.5
      P2G=PCR*TR2*(-W1(TR2)*RHR21**2-W2(TR2)*RHR21**3+G(RHR21))
  290 RHR22=1.03*RHR21
      FROJ=SFROJ(T3P,P3P,RH3P,T2,P2G)
      FTR2=FTR(TR3P,TR2,RHR3P,RHR22)
      FTR1=FTR(TR3P,TR2,RHR3P,RHR21)
      RHR22=-(RHR22-RHR21)*FTR1/(FTR2-FTR1)+RHR21
      IF (ABS(FTR(TR3P,TR2,RHR3P,RHR22)).LE..000005) GO TO 300
      RHR21=RHR22
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```
      GO TO 290
  300 RHR2=RHR22
      RH2=RHR2*RHCR
      P2=PCR*TR2*(-W1(TR2)*RHR2**2-W2(TR2)*RHR2**3+G(RHR2))
      IF (ABS(P2-P2G).LE..1) GO TO 310
      P2G=P2
      GO TO 290
  310 P6=P2
      IF (THIGH.GE.TOPR) GO TO 120
      IF (NOS.EQ.1) GO TO 120
  320 CONTINUE
      PHIGH=P2
      PR2=P2/PCR
      T6=TBL/(1.-ALOG(P2/14.7)*(1.-TBL/TCR)/ALOG(PCR/14.7))
      TR6=T6/TCR
      TKH=5.*T6/9.
      IF (NO.EQ.2) GO TO 330
      DHT=((P3P/RH3P)-(P2/RH2))*144./AJ+(CP0-FROJ)*(T3P-T2)+CP1*(T3P**2-
     1T2**2)/2.+CP2*(T3P**3-T2**3)/3.+ZC*R*T2*(-((AKO/TR2)+(2.*AW1/TR2**
     22))*(RHR3P-RHR2)+(AW2*(RHR3P**2-RHR2**2)/(TR2**2)))/AJ
      DHR=-DHT*(1.-ETT)
  330 CONTINUE
      DHSH=CP0*(T2-T6)+CP1*(T2**2-T6**2)/2.+CP2*(T2**3-T6**3)/3.
      DHBLH=CPL0*(T6-TLOW)+CPL1*(T6**2-TLOW**2)/2.
     1+CPL2*(T6**3-TLOW**3)/3.
      TR=TR6
      PR=PR2
      RH2P=RH3P
  340 DHBV=454.*TKH*DHCM(TR,PR)/(252.*GPGM)
  350 CONTINUE
      VL=(2.*TKCR-TKB)/(RHCR*(.422*ALOG10(PCR/14.7)+1.981)*(2.*TKCR-TKL)
     1)
      DHPW=VL*144.*(PHIGH-PLOW)/AJ
      BG=-DHT
      VEL=ETN*SQRT(2.*AGC*AJ*BG)
      AMDOT=3413.*EPR/(ETGN*(-DHT*ETT-DHPW/ETP))
      PW=VL*(PHIGH-PLOW)*AMDOT*.0000727/ETP
      PFR=VL*AMDCT*.125
      TFR=AMDOT/(RH2P*60.)
      FNS=(60.*VEL*SQRT(TFR/60.))/(2.*3.1416*(AJ*BG)**.75)
      DS=((AJ*BG)**.25)/(SQRT(TFR/60.))
      TR=TKC/TKCR
      PR=PLOW/PCR
      DHC=((454.*TKC)/(252.*GPGM))*DHCM(TR,PR)
      IF (NO.EQ.1) GO TO 360
      BH=(DHBLH+DHBV+DHSH-DHPW/ETP)*AMDOT
      BLH=(DHBLH-DHPW/ETP)*AMDOT
      BVH=DHBV*AMDOT
      BSH=DHSH*AMDOT
      GO TO 370
  360 BH=(-DHT*ETT+DHR+DHC-DHPW/ETP)*AMDOT
  370 CONTINUE
      CH=(DHC+(1.-ETR)*DHR)*AMDOT
      RH1=DHR*AMDOT
      RH=DHR*ETR*AMDOT
      BH1=BH-RH
      SH=DHSH*AMDOT
```

```
      EFF1=(ETGN*(-ETT*DHT-DHPW/ETP))*100./(BH/AMDOT)
      EFF2=(ETGN*(-ETT*DHT-DHPW/ETP))*100./(BH1/AMDOT)
      EFFC=100.*(1.-TLOW/THIGH)
      IF (NO.EQ.4) T2P=T3P
      RADHT=-DHT*(1.-ETT)
      T2P1=T2P+15.
 380  T2P2=T2P1+5.
      RADHT1=CP0*(T2P1-T2P)+CP1*(T2P1**2-T2P**2)/2.+CP2*(T2P1**3-T2P**3)
     1/3.-RADHT
      RADHT2=CP0*(T2P2-T2P)+CP1*(T2P2**2-T2P**2)/2.+CP2*(T2P2**3-T2P**3)
     1/3.-RADHT
      T2P2=-(T2P2-T2P1)*RADHT1/(RADHT2-RADHT1)+T2P1
      EROR=-RADHT+CP0*(T2P2-T2P)+CP1*(T2P2**2-T2P**2)/2.+CP2*(T2P2**3-T2
     1P**3)/3.
      IF (ABS(EROR).LE..00001) GO TO 390
      T2P1=T2P2
      GO TO 380
 390  CONTINUE
      T2PS=T2P
      T2PSP=T2PS-459.69
      TR2PS=T2PS/TCR
      TRHIGH=THIGH/TCR
      PRHIGH=PHIGH/PCR
      W1T=W1(TRHIGH)
      W2T=W2(TRHIGH)
      RHIGH=(RHO(PRHIGH,TRHIGH,W1T,W2T))
      RRHIGH=RHIGH/RHCR
      PRLOW=PLOW/PCR
      W1T=W1(TR2PS)
      W2T=W2(TR2PS)
      RRLOW=(RHO(PRLOW,TR2PS,W1T,W2T))/RHCR
      DH1HT=DHHO(TRHIGH,RRHIGH)+DHT/(1.-(RRHIGH*A1A2/RRLOW)**2)
      EX=1./(1.-(ALOG(T2PS/THIGH))/(ALOG(PLOW/PHIGH)))
      TT1=THIGH*2./(EX+1.)
      TRT1=TT1/TCR
      RHRT1=RRHIGH*(2./(EX+1.))**(1./(EX-1.))
 392  RHRT2=1.03*RHRT1
      PT=PCR*TRT1*(-W1(TRT1)*RHRT1**2-W2(TRT1)*RHRT1**3
     1+G(RHRT1))
      TT1=TRT1*TCR
      FROJ=SFROJ(THIGH,PHIGH,RHIGH,TT1,PT)
      FTR1=FTR(TRHIGH,TRT1,RRHIGH,RHRT1)
      IF(ABS(FTR1).LE..00001) GO TO 394
      FTR2=FTR(TRHIGH,TRT1,RRHIGH,RHRT2)
      RHRT1=RHRT1-(RHRT2-RHRT1)*FTR1/(FTR2-FTR1)
      IF(RHRT1.GE.0.0) GO TO 392
      RHRT1=RHRT2/2.
      GO TO 392
 394  CONTINUE
      TRT2=1.03*TRT1
      ERDH1A = (C2(TRT1,RHRT1))/(2.*AGC*AJ)
      ERDH1 = ERDH1A - DH1HT + DHHO(TRT1,RHRT1)
      IF(ABS(ERDH1).LE..0001) GO TO 396
      ERDH2A = (C2(TRT2,RHRT1))/(2.*AGC*AJ)
      ERDH2 = ERDH2A - DH1HT + DHHO(TRT2,RHRT1)
      TRT1=TRT1-(TRT2-TRT1)*ERDH1/(ERDH2-ERDH1)
      IF(TRT1.GE.0.0) GO TO 394
```

```
      TRT1=TRT2/2.
      GO TO 394
 396  TDUM=TRT1*TCR
      IF(ABS(TDUM-TT1).GE.1.) GO TO 392
      C=SQRT(C2(TRT1,RHRT1))
      ANT=144.*AMDOT/(ETN*RHRT1*RHCR*C*3600.)
      C=SQRT(C2(TR2PS,RRLOW))
      ANE=144.*AMDOT/(VEL*RRLOW*RHCR*3600.)
      FM=VEL/(ETN*C)
      T2P=T2P2
      IF (NO.EQ.1) GO TO 420
      IF (NO.EQ.2) GO TO 420
      IF (SDSDT.GE.0.0) GO TO 410
      PRINT*,1H
      PRINT*,≠ SUB-CRITICAL WETTING FLUID CYCLE≠
      T6PT=T6-459.69
      T2PT=T2-459.69
      T3PT=T3P-459.69
      T2PP=T2P-459.69
      PRINT 830, T6PT, P6
 830  FORMAT (2X,≠BOILER TEMP =≠,F6.1,1X,≠DEGREES F≠
     1  ,6X,≠BOILER PRESSURE =≠,F7.2,1X,≠PSIA≠)
      PRINT 750, T2PT
 750  FORMAT (2X,≠SUPERHEAT TEMPERATURE =≠,F10.2,1X,≠DEGREES F≠)
      PRINT 822, T2PSP
 822  FORMAT (2X,≠NOZZLE EXIT TEMP(ISENTROPIC) =≠,
     1F7.3,1X,≠DEGREES F≠)
      PRINT 820, T2PP
 820  FORMAT (2X,≠TURBINE EXHAUST TEMP =≠,F7.2,1X,≠DEGREES F≠)
      PRINT 822, T2PSP
      PRINT 810, T3PT, P3P
 810  FORMAT (2X,≠COND TEMP =≠,F7.2,1X,≠DEGREES F≠,4X,≠COND PRESSURE =≠,
     1F7.2,1X,≠PSIA≠)
      GO TO 430
 400  CONTINUE
      T6P=T6-459.69
      PRINT 830, T6P, PHIGH
      GO TO 430
 410  T1PP=T1P-459.69
      T3P=T3-459.69
      T2PP=T2P-459.69
      PRINT 780
 780  FORMAT ( /,2X,≠SUB-CRITICAL DRYING FLUID CYCLE≠)
      PRINT 830, T1PP, P1P
      PRINT 810, T3P, P3
      PRINT 822, T2PSP
      PRINT 820, T2PP
      GO TO 430
 420  THIGHP=THIGH-459.69
      T2PP=T2P-459.69
      TLOWP=TLOW-459.69
      PRINT 850, THIGHP, PHIGH
 850  FORMAT (2X,≠SUPERHEAT TEMP =≠,F6.1,1X,≠DEGREES F≠,
     12X,≠SUPERHEAT PRESSURE =≠,F7.2,1X,≠PSIA≠)
      PRINT 822, T2PSP
      PRINT 820, T2PP
      PRINT 810, TLOWP, PLOW
```

```
      IF (NO.EQ.2) GO TO 400
  430 PRINT 700, VEL
 700  FORMAT (2X,≠NOZZLE SPOUTING VEL =≠,F7.2,1X,≠ FT/SEC≠ )
      PRINT 701, FM
 701  FORMAT(2X,≠NOZZLE EXIT MACH NUMBER(ISENTROPIC) =≠,F5.3 )
      PRINT 702, ANT
 702  FORMAT (2X,≠NOZZLE THROAT AREA =≠,G12.6,1X,≠SQUARE INCHES≠)
      PRINT 704, ANE
 704  FORMAT (2X,≠NOZZLE EXIT AREA =≠,G12.6,1X,≠SQUARE INCHES≠)
      PRINT 710, PW
 710  FORMAT (2X,≠BOILER FEED PUMP =≠,G11.5,1X,≠HP≠)
      PRINT 720, AMDOT
 720  FORMAT (2X,≠MASS FLOW RATE =≠,G12.6,1X,≠LBM/HR≠)
      PRINT 730, PFR
 730  FORMAT (2X,≠PUMP VOLUMETRIC FLOW =≠,G11.5,1X,≠GAL/MIN≠)
      PRINT 740, TFR
 740  FORMAT (2X,≠TURBINE EXHAUST FLOW =≠,G12.6,1X,≠CUBIC FT/MIN≠)
      PRINT 570, BG
 570  FORMAT (2X,≠TURBINE ISENTROPIC HEAD =≠,G11.5,1X,≠BTU/LBM≠)
      PRINT 550, FNS
 550  FORMAT (2X,≠TURBINE SPECIFIC SPEED ( ROTOR DIA.= 1 FT.) =≠,G10.4)
      PRINT 560, DS
      PRINT 650, BH
  560 FORMAT(2X,≠TURBINE SPECIFIC DIAMETER ( ROTOR DIA.=1 FT.) =≠,G10.4)
 650  FORMAT (2X,≠BOILER HEAT RATE (NO REGENERATION) =≠,
     1G14.8,1X,≠BTU/HR≠)
      IF (NO.EQ.1) GO TO 440
      PRINT 860, BLH
 860  FORMAT (5X,≠OF WHICH ≠,G14.6,≠ BTU/HR IS HEAT≠
     1 ,≠ ADDED TO LIQUID≠ )
      PRINT 870, BVH
 870  FORMAT (14X,G14.8,≠ BTU/HR IS FOR VAPORIZATION≠)
      PRINT 880, BSH
 880  FORMAT (14X,G14.8,≠ BTU/HR IS FOR SUPERHEATING≠)
 440  CONTINUE
      PRINT 660, BH1
 660  FORMAT (2X,≠BOILER HEAT RATE (WITH REGENERATION) =≠
     1    ,G14.8,1X,≠BTU/HR≠)
      PRINT 670, CH
 670  FORMAT (2X,≠CONDENSER HEAT RATE(WITH REGENERATION) =≠,G14.6,1X,≠BT
     1U/HR≠)
      PRINT 680, RH1
 680  FORMAT (2X,≠REGENERATOR HEAT RATE(VAPOR SIDE)=≠,
     1G14.8,1X,≠BTU/HR≠)
      PRINT 690, RH
 690  FORMAT (2X,≠REGENERATOR HEAT RATE(LIQUID SIDE) =≠,G14.8,1X,≠BTU/HR
     1≠)
C  CALCULATE THE REGENERATOR LIQUID OUTPUT TEMPERATURE
      A = DHPW*(1.0-ETP)/ETP + DHR*ETR
      ITER = 0
      CONST = A +TLOW*(CPL0 +CPL1*TLOW/2. +CPL2*TLOW*TLOW/3.)
      X = TAVE
 1000 ITER = ITER +1
      FOX = X*(CPL0 + .5*CPL1*X + CPL2*X*X/3.) - CONST
      DFOX = CPL0 + X*(CPL1 + CPL2*X)
      XOLD = X
      X = XOLD - FOX/DFOX
```

```
      IF(ABS(X-XOLD) .LT. ( .0001*X) ) GO TO 1010
      IF(ITER .LT. 20) GO TO 1000
      PRINT*,≠ ITERATION FOR REGEN TEMP NOT CONVERVING≠
      GO TO 450
 1010 TOREG =  X - 459.69
      PRINT 1020,TOREG
 1020 FORMAT(2X,≠TEMP OF LIQUID OUTPUT FROM REGENERATOR = ≠
     1 ,G11.5, ≠ DEGREES F≠ )
      PRINT 840, SH
 840  FORMAT (2X,≠SUPERHEATER HEAT RATE =≠,1X,G14.8,1X,≠BTU/HR≠)
      PRINT 760, EFF1
 760  FORMAT (2X,≠EFFICIENCY (WITHOUT REG)=≠,F5.1,1X,≠%≠)
      PRINT 790, EFF2
 790  FORMAT (2X,≠EFFICIENCY (WITH REG)=≠,F5.1,1X,≠%≠)
      PRINT 800, EFFC
 800  FORMAT (2X,≠CARNOT EFFICIENCY =≠,F5.1,1X,≠%≠////)
  450 PRINT*,≠ ANY MORE TEMPERATURES≠,
      READ(1,48) IQ
      IF(EOF(1)) 455,456
  455 IQ = 2HNO
  456 NO=0
      NOS=0
      IF(IQ .EQ. 3HYES) GO TO 40
C
      END
```

```
FUNCTION RHO          74/74    OPT=0  TRACE

      FUNCTION RHO (P,T,W1T,W2T)
      COMMON AR1,AR2,AR3,AR4,RHCR,R
      COMMON AKO,AW1,AW2,ZC,AJ,AGC
      COMMON /FLUID/ BETA,ALPHC,CP0,CP1,CP2,TCR,PCR,TBL,GPGM
      RH1=(P*PCR*144.)/(R*T*TCR*RHCR)
   10 RH2=1.05*RH1
      EHBMS1=-W1T*RH1**2-W2T*RH1**3+(AR1*RH1)/(AR2-AR3*RH1+AR4*RH1**2)-P
     1/T
      EHBMS2=-W1T*RH2**2-W2T*RH2**3+(AR1*RH2)/(AR2-AR3*RH2+AR4*RH2**2)-P
     1/T
      RH3=-((RH2-RH1)/(EHBMS2-EHBMS1))*EHBMS1+RH1
      IF (RH3.GE.0.0) GO TO 20
      RH3=RH1/2.
   20 CONTINUE
      EHBMS3=-W1T*RH3**2-W2T*RH3**3+(AR1*RH3)/(AR2-AR3*RH3+AR4*RH3**2)-P
     1/T
      IF (ABS(EHBMS3).LE..000005) GO TO 30
      RH1=RH3
      GO TO 10
   30 RHO=RH3*RHCR
      RETURN
C
      END
```

```
FUNCTION SFROJ       74/74    OPT=0  TRACE

      FUNCTION SFROJ (T1P,P1P,RH1P,T2P,P2P)
      COMMON AR1,AR2,AR3,AR4,RHCR,R
      COMMON AKO,AW1,AW2,ZC,AJ,AGC
      COMMON TOPR,POPR
      COMMON /FLUID/ BETA,ALPHC,CP0,CP1,CP2,TCR,PCR,TBL,GPGM
      ARH1P=RH1P
      IF (ABS(T1P-TCR).GE.ABS(TCR-TOPR)) GO TO 10
      IF (P1P.LE.POPR) GO TO 10
      TR1P=T1P/TCR
      AP1P=POPR
      PR1P=AP1P/PCR
      W1T=AKO/TR1P+AW1/TR1P**2
      W2T=AW2*(1.-1./TR1P**2)
      ARH1P=RHO(PR1P,TR1P,W1T,W2T)
   10 CONTINUE
      TR=T2P/TCR
      W1T=AKO/TR+AW1/TR**2
      W2T=AW2*(1.-1./TR**2)
      P=P2P/PCR
      T=T2P/TCR
      RH2P=RHO(P,T,W1T,W2T)
      PTE=ALOG(RH2P/ARH1P)/ALOG(T2P/T1P)
      DT=(T1P-T2P)/20.
      SMFN=0.0
      DO 20 I=1,21
      T=T1P-(I-1)*DT
      RH=ARH1P*(T/T1P)**PTE
      TR=T/TCR
      RHR=RH/RHCR
      DPDT=(AW1*RHR**2)/TR**2-AW2*(RHR**3)*(TR**2+1.)/TR**2+AR1
     1*RHR/(AR2-AR3*RHR+AR4*RHR**2)
      DPDRH=-2.*TR*(AKO/TR+AW1/TR**2)*RHR-3.*AW2*(RHR**2)*(TR**2-1.)/TR+
     1TR*AR1*(AR2-AR4*RHR**2)/(AR2-AR3*RHR+AR4*RHR**2)**2
      A=1
      IF (I.EQ.1) A=2.
      IF (I.EQ.21) A=2.
      SMFN=SMFN+(DT/A)*ZC*TR*(DPDT**2)/(DPDRH*RHR**2)
   20 CONTINUE
      SFROJ=(SMFN*R)/((T1P-T2P)*AJ)
      RETURN
      END
```

APPENDIX C

The fluid input constants required by CYCLE are listed below in the order in which they appear in the fluid data files.

1. BETA (or β) - a parameter defined in terms of the critical compressibility, i. e.,

$$Z_c = \frac{MP_cV_c}{RT_c} = \frac{\beta(3\beta - 1)}{(1 + \beta)^3}$$

   A table of β vs. Z_c can be found in Reference 9.

2. ALPHC (or α) - the slope of the vapor pressure curve at the critical point, commonly referred to as the Riedel constant.

3. CP0, CP1 and CP2 - constants in the equation for the specific heat of the working fluid. See Eq. (7-1). These constants are found by curve fitting the tabulated change in enthalpy vs. temperature at any constant pressure representative of the pressures encountered in the range of calculations to be performed.

4. TCR (or T_c) - critical temperature.

5. PCR (or P_c) - critical pressure.

6. TBL (or T_b) - normal ($P = 14.696$ lb/in^2) boiling temperature.

7. GPGM (or M) - molecular weight.

8. CPL0, CPL1, CPL2 - same as 3 except for the liquid phase. See Eq. (10-1).

The required fluid data can be found in sources such as steam tables, chemical manufacturer's publications, handbooks, etc. Where tabulated data is not available, Reference 10 contains numerous methods of estimating the required parameters.

Data files for several fluids being evaluated for use in Sandia's Solar Community studies are listed below.

a. Water (H_2O)

```
/list,fn=wat

9.096E0,7.402E0,4.271E-1,1.009E-5,3.518E-8,1.165E3
3.206E3,6.717E2,1.802E1,2.200E0,-3.658E-3,2.754E-6
```

b. Toluene ($CH_3C_6H_5$)

```
list,fn=tol

7.48E00,7.096E00,-6.823E-2,7.274E-4,-1.818E-7,1.0651E3
5.959E2,6.908E2,9.213E1,4.195E-1,-4.669E-4,7.663E-7
```

c. **Chlorobenzene (C_6H_5Cl)**

```
list,fn=chl
```

```
7.385E0,7.022E0,-5.168E-2,5.760E-4,-1.758E-7,1.138E3
6.554E2,7.288E2,1.126E2,7.346E-2,3.819E-4,3.893E-8
```

d. **Benzene (C_6H_6)**

```
list,fn=ben
```

```
6.975E0,6.838E0,-9.801E-2,7.600E-4,-2.057E-7;1.012E3
7.104E2,6.359E2,7.811E1,6.689E-1,-1.298E-3,1.433E-6
```

e. **Thiophene (C_4H_4S)**

```
list,fn=thi
```

```
7.701E0,6.761E0,-7.228E-2,6.257E-4,-2.025E-7,1.043E3
8.259E2,6.431E2,8.414E1,9.478E-1,-2.118E-3,1.837E-6
```

f. **Pyridine (C_5H_5N)**

```
list,fn=pyr
```

```
6.839E0,6.987E0,-1.164E-1,7.721E-4,-2.284E-7,1.116E3
8.171E2,6.997E2,7.910E1,4.777E-1,-6.906E-4,8.986E-7
```

g. **Refrigerant 11 (CCl_3F)**

```
list,fn=r11
```

```
6.850E0,6.740E0,7.124E-2,1.635E-4,-7.002E-8,8.482E2
6.350E2,5.351E2,1.374E2,5.181E-1,-1.133E-3,1.040E-6
```

h. Refrigerant 12 (CCl_2F_2)

```
list,fn=r12

7.015E0,6.660E0,4.796E-2,2.344E-4,-1.013E-7,6.933E2
5.970E2,4.381E2,1.209E2,1.030E0,-3.320E-3,3.412E-6
```

i. Trifluoroethanol (CF_3CH_2OH)

```
list,fn=tri

8.293E0,6.804E0,6.610E-2,3.694E-4,-1.059E-7,8.997E2
7.150E2,6.242E2,1.000E2,2.395E0,-6.427E-3,5.226E-6
```

j) Ammonia (NH_3)

```
list,fn=amm

8.550E0,7.000E0,1.416E0,-2.766E-3,2.193E-6,7.311E2
1.654E3,4.316E2,1.703E1,8.523E-1,2.870E-6,1.010E-6
```

k) Hexafluorobenzene (C_6F_6)

```
list,fn=hex

7.884E0,7.755E0,6.187E-2,3.163E-4,-1.041E-7,9.300E2
4.748E2,6.359E2,1.861E2,3.475E-1,-4.171E-4,5.325E-7
```

l) Isobutane ($CH(CH_3)_3$)

```
list,fn=iso

6.536E0,6.699E0,8.789E-2,6.327E-4,-3.995E-8,7.347E2
5.291E2,4.707E2,5.812E1,1.642E0,-4.475E-3,4.722E-6
```

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