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A Method for Calculating the Steady-State Distribution of Tritium in a Molten-Salt Breeder Reactor Plant

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A METHOD FOR CALCULATING THE STEADY-STATE DISTRIBUTION OF TRITIUM IN A MOLTEN-SALT BREEDER REACTOR PLANT

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A METHOD FOR CALCULATING THE STEADY-STATE DISTRIBUTION OF TRITIUM IN A MOLTEN-SALT BREEDER REACTOR PLANT

R. B. Briggs and C. W. Nestor, Jr.

ABSTRACT

Tritium is produced in molten salt reactors primarily by fissioning of uranium and absorption of neutrons by the constituents of the fuel carrier salt. At the operating temperature of a large power reactor, tritium is expected to diffuse from the primary system through pipe and vessel walls to the surroundings and through heat exchanger tubes into the secondary system which contains a coolant salt. Some tritium will pass from the secondary system into the steam power system. This report describes a method for calculating the steady state distribution of tritium in a molten salt reactor plant and a computer program for making the calculations. The method takes into account the effects of various processes for removing tritium, the addition of hydrogen or hydrogenous compounds to the primary and secondary systems, and the chemistry of uranium in the fuel salt. Sample calculations indicate that 30 percent or more of the tritium might reach the steam system in a large power reactor unless special measures are taken to confine the tritium.

I. INTRODUCTION

Conceptual designs of Molten Salt Breeder Reactor (MSBR) power plants usually can be represented by the diagram shown in Fig. 1. The fissioning of uranium in the fuel salt heats the salt as it is pumped through the reactor vessel in the primary system. The heat is transferred to a coolant salt that circulates in the secondary system and, thence, to water, producing steam to drive a turbine-generator in the steam system.

Fission products and other radioactive materials are produced in large amounts in the fuel salt. Much smaller amounts are produced in the coolant salt by the flux of delayed neutrons in the primary heat exchangers. The radioactivity is normally confined by the walls of the piping and vessels. However, tritium is produced in the salts, partly as a fission product, but mostly by absorption of neutrons by lithium in the fuel salt. At the high temperature of an MSBR, tritium diffuses through metals and might escape to the environs in amounts that would be cause for concern.

The purpose of this report is to describe a method for calculating the distribution of tritium in and its escape from an MSBR plant. We assume that the tritium, born as tritium ions, is present in the fuel salt primarily as tritium molecules* and tritium fluoride molecules.** The ions are estimated to be produced at a rate of 2.6×10^{14}/MWsec***

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*Tritium molecules are intended to include HT and H_2 molecules when hydrogen is present.

**Tritium fluoride molecules are intended to include tritium (and hydrogen) ions associated with fluoride ions in the salt.

***2420 Ci/day in a 2250 MW(t), 1000 MW(e) plant.

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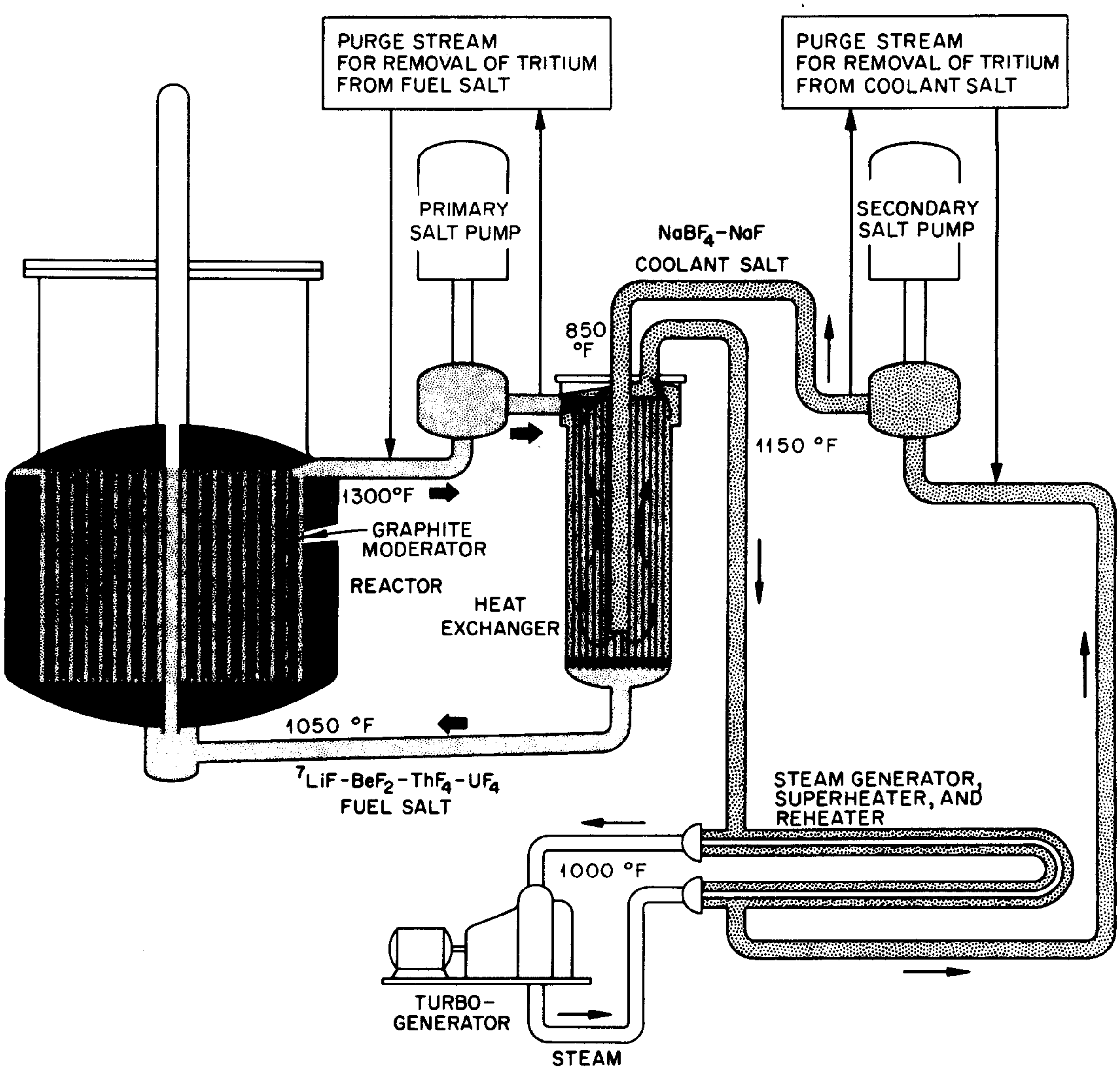

Fig. 1. Molten Salt Breeder Reactor System.

in a typical fuel salt. The relative concentrations of tritium and tritium fluoride in the fuel salt are expected to be governed by the equilibrium relationship for the reaction,

$$UF_4 + 1/2\ T_2 \rightleftarrows UF_3 + TF\ ,$$

with uranium in the salt. The absolute concentrations are governed by removal processes.

Three types of processes are provided for removing tritium from the primary system: permeation through the metal of the walls of piping and vessels, sorption on materials in contact with the salt, and purging. We assume that tritium molecules that reach a metal surface can sorb on the surface, dissociate into tritium atoms and diffuse through the metal. Tritium in tritium fluoride and other compounds is assumed to be chemically bound and unable to pass through the metal.

Experience with the Molten Salt Reactor Experiment indicated that tritium sorbs on and is tightly bound to graphite. We provide for sorption of tritium and tritium fluoride on the graphite in the reactor core.

Provision is made for purging tritium from the primary system by circulating a stream of salt through an apparatus which extracts gaseous tritium and tritium compounds. A contactor in which tritium and tritium fluoride are transferred to a gas phase by virtue of their vapor pressures would be such an apparatus. Current designs for MSBR's provide for sparging of the fuel salt with helium bubbles in the primary system to remove krypton and xenon. Tritium and tritium fluoride would be removed also. The sparging process can be treated as an equivalent purging process in the calculations.

Tritium will reach the secondary system by diffusion from the primary system through the walls of the tubes in the primary heat exchangers and by neutron capture in the coolant salt. We provide for removal of tritium from the secondary system by diffusion through the metal walls, sorption, and purging. The secondary system would not normally contain a sorber or have an elaborate purging system. Such processes, if incorporated into the plant, would be designed specifically for removing tritium.

The coolant salts do not normally contain constituents that are reducible by tritium and, thereby, able to convert tritium into tritium fluoride and make it unavailable to diffuse through the metal walls. We, therefore, have provided for addition of hydrogen fluoride or other hydrogenous compounds to the secondary system. We assume that tritium will exchange with the hydrogen in the added compound and that the compound will be extracted by the sorption and/or purge process.

The steam system and the cells around the reactor primary and secondary systems are considered to be sinks for tritium. Tritium reaching the steam system is assumed to exchange with hydrogen in the water, and that reaching the cells is assumed to be oxidized to water. The partial pressure of tritium is effectively zero.

In the calculations we assume that tritium and hydrogen behave identically. The equation used for calculating the diffusion of hydrogen through a metal wall states that the rate of transport per unit of surface area is proportional to the product of a permeability coefficient and the difference between the square roots of the partial pressures of hydrogen at the inner and outer surfaces of the metal.

In this circumstance, addition of hydrogen can reduce the transport of tritium through the metal. Suppose, for example, the partial pressures of tritium and hydrogen at the outer surface of a pipe are zero and the partial pressure of tritium at the inner surface is held constant. If hydrogen were added to increase the total hydrogen partial pressure at the inner surface by a factor of 100, the flow of hydrogen plus tritium through the metal wall would increase by a factor of 10. But the flow of tritium would decrease by a factor of 10 because of the 100-fold dilution of hydrogen. Because of other factors, the effect of adding hydrogen may not be so dramatic, but the calculational method provides for addition of hydrogen to the primary and secondary systems and for hydrogen to be present at a specified concentration in the steam system so that the effects can be studied.*

The calculational model describes the behavior of tritium in an MSBR plant to the extent that it is known or has been inferred at the present time. The removal processes can be included in or eliminated from the calculations by careful choice of the values assigned to coefficients in the equations. The model probably does not include all the chemical reactions and physical processes that will ultimately be

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*The calculational procedure might have been developed to treat hydrogen and tritium as separate species. Separate values then could be assigned to important parameters, such as solubility and diffusion coefficients, for each species. Interaction between hydrogen and tritium would be taken into account by the equilibrium relationship

$$p_{HT}^2/p_{H2} \bullet p_{T2} = k_p \text{ for the reaction } H_2 + T_2 \rightleftarrows HT \ .$$

However, k_p has a value near 4 at temperatures of interest, which signifies that hydrogen and tritium interact as though they are the same species. Also, there are substantial uncertainties in the values for most of the parameters. Complicating the procedure to treat hydrogen and tritium separately would not, for the present, improve the accuracy of the results.

shown to affect the distribution of tritium in an MSBR. In some instances these effects can be included, when recognized, simply by adjusting the coefficients in equations for processes presently included. Others may require incorporation of additional processes.

Two assumptions in the calculational procedure should be recognized for their potential for leading to major differences between the calculated distribution of tritium and what would actually occur in a reactor plant. Tritium, present in the salt as tritium fluoride, can react with metal to yield tritium atoms that would dissolve in and diffuse through the metal. Neglect of this reaction could cause the calculations to be greatly in error under circumstances where most of the tritium is present in the salt as tritium fluoride.

Oxide films (and possibly others) that form on metal surfaces reduce the permeability of a metal wall to the passage of hydrogen. They may also cause the transport to vary with pressure to a power in the range of 1/2 to 1. The reduced permeability appears as a coefficient in the transport equations of the model, but we make no provision for changing the exponent on the pressure terms from 1/2. The calculated transport of tritium through the metal walls and the effect of the addition of hydrogen in reducing the transport would both be greater than would actually occur if the actual transport were proportional to the pressure to a power in the range 1/2 to 1. The calculations would not underestimate the transport unless the total pressure of tritium and hydrogen exceeded the reference pressure for the permeability coefficient, which is usually 1 atm.

II. DERIVATION OF EQUATIONS AND COMPUTATIONAL PROCEDURES

In making the calculations, we first calculate the distribution of hydrogen plus tritium in order to establish flows and concentrations of the combined isotopes throughout the plant. Then we calculate the distribution of tritium throughout the plant.

For calculating the distribution, the fluids in the primary and secondary systems and the various parts of the steam system are assumed to be well mixed and to contain uniform bulk concentrations of all constituents. The calculations are for steady-state conditions, and only hydrogen and tritium molecules are assumed to be able to sorb on the metal surfaces, dissociate, and diffuse through the metal walls. The various paths are defined and the distribution is calculated by the use of the following set of equations.*

A. In the primary system:

1. Transport of hydrogen through the salt film to the wall of the piping in the hot leg from the reactor vessel to the heat exchanger:

$$Q_1 = h_1 A_1 (C_F - C_1) \ . \tag{1a}$$

Transport through the pipe wall to the surroundings where the hydrogen pressure is assumed to be negligible:

$$Q_1 = \frac{p_1 A_1 \left[(k_1 C_1)^{\frac{1}{2}} - 0\right]}{t_1} = \frac{p_1 A_1 (k_1 C_1)^{\frac{1}{2}}}{t_1} \ . \tag{1b}$$

2. Transport of hydrogen to and through the walls of the cold-leg piping from the heat exchanger to the reactor vessel:

---

*Symbols are defined in Section IV, Nomenclature.

$$Q_2 = h_2A_2(C_F - C_2) \quad (2a)$$

$$= \frac{p_2A_2(k_2C_2)^{\frac{1}{2}}}{t_2} . \quad (2b)$$

3. Transport of hydrogen to and through the walls of the reactor vessel and the shells of the heat exchangers in the primary system:

$$Q_3 = h_3A_3(C_F - C_3) \quad (3a)$$

$$= \frac{p_3A_3(k_3C_3)^{\frac{1}{2}}}{t_3} \quad (3b)$$

4. Transport of hydrogen to and through the walls of the tubes in the primary heat exchangers into the secondary system:

$$Q_4 = h_4A_4(C_F - C_4) \quad (4a)$$

$$= \frac{p_4A_4}{t_4}\left[(k_4C_4)^{\frac{1}{2}} - (k_{12}C_{12})^{\frac{1}{2}}\right] . \quad (4b)$$

5. Transport of hydrogen to the surfaces of the graphite in the reactor vessel or to other sorber:

$$Q_5 = h_5A_5(C_F - C_5) . \quad (5a)$$

Sorption by the graphite or other sorber assuming that the sorbing surface is replaced continuously and that the concentration of sorbed gas is proportional to the square root of the partial pressure:

$$Q_5 = B_1W_1A_5(k_5C_5)^{\frac{1}{2}} . \quad (5b)$$

6. Removal of hydrogen by purge:

$$Q_6 = F_1E_1C_F . \quad (6)$$

7. Transport of hydrogen fluoride to and removal by sorber:

$$Q_7 = h_7 A_7 (C_{FF} - C_7) \quad (7a)$$

$$= B_2 W_2 A_7 (k_7 C_7)^{\frac{1}{2}} \; . \quad (7b)$$

8. Removal of hydrogen fluoride by purge:

$$Q_8 = F_2 E_2 C_{FF} \; . \quad (8)$$

Because the molecular species involved may contain different numbers of hydrogen atoms, all the calculations are done in terms of atoms of hydrogen. This does not mean that the hydrogen necessarily diffuses as single atoms, but only that a transport unit is one hydrogen atom and the parameters are expressed in terms of single hydrogen atoms. A Q value of 1 then represents the transport of one-half molecule of H_2, one molecule of HF, or one-fourth molecule of a compound like CH_4, all per unit time. Likewise, a C value of 1 represents a concentration of one-half molecule of H_2, one molecule of HF, or one-fourth molecule of CH_4, all per unit volume.

If the rates of inflow of tritium and hydrogen atoms (R_1 and R_2, respectively) to the primary system are given, a material balance over the primary system gives

$$R_1 + R_2 = \sum_{i=1}^{8} Q_i \; . \quad (9)$$

In our calculations, all flow rates in the sum on the right-hand side of Eq. 9 are positive or zero except for Q_4, the transport through the heat exchanger tubes to the secondary system. Q_4 can be positive, negative or zero, depending on the conditions in the various systems. Hydrogen is present in and is removed from the primary system as hydrogen fluoride, but we provide no input of HF. It is produced by the reaction

$$UF_4 + \tfrac{1}{2}H_2 \rightleftarrows UF_3 + HF \ ,$$

which has an equilibrium quotient

$$\frac{X(UF_3)}{X(UF_4)} \times \frac{P(HF)}{[P(H_2)]^{\frac{1}{2}}} = M' \ ,$$

or

$$\frac{X(UF_3)}{X(UF_4)} \times \frac{k_7 C_{FF}}{(k_5 C_F)^{\frac{1}{2}}} = M \ .$$

Corrosion and other chemical considerations make it desirable to maintain the ratio $X(UF_3)/X(UF_4) \equiv 1/U$ at a constant value,* so the concentration of HF in the bulk of the salt can be related to the hydrogen concentration by

$$C_{FF} = \frac{MU}{k_7} \left(k_5 C_F\right)^{\frac{1}{2}} \ . \tag{10}$$

We replace C_{FF} by the equivalent function of C_F in Eqs. 7a and 8 to obtain expressions for Q_7 and Q_8 in terms of C_F.

B. Secondary System:

1. Hot-leg piping:

$$Q_{10} = h_{10} A_{10} (C_C - C_{10}) \tag{11a}$$

$$= \frac{p_{10} A_{10}}{t_{10}} (k_{10} C_{10})^{\frac{1}{2}} \ . \tag{11b}$$

---

*This might require that hydrogen be added to the primary systems as a mixture of hydrogen and hydrogen fluoride.

2. Cold-leg piping:

$$Q_{11} = h_{11}A_{11}\ (C_C - C_{11}) \tag{12a}$$

$$= \frac{p_{11}A_{11}}{t_{11}}\ (k_{11}C_{11})^{\frac{1}{2}}\ . \tag{12b}$$

3. Transport through the primary heat exchanger tubes into the primary system:

$$Q_{12} = h_{12}A_4\ (C_C - C_{12}) \tag{13a}$$

$$= \frac{p_4A_4}{t_4}\left[(k_{12}C_{12})^{\frac{1}{2}} - (k_4C_4)^{\frac{1}{2}}\right]\ . \tag{13b}$$

4. Transport through the steam generator tubes into the steam system:

$$Q_{13} = h_{13}A_{13}\ (C_C - C_{13}) \tag{14a}$$

$$= \frac{p_{13}A_{13}}{t_{13}}\ \left[(k_{13}C_{13})^{\frac{1}{2}} - (k_{21}C_{21})^{\frac{1}{2}}\right]\ . \tag{14b}$$

5. Transport through the superheater tubes into the steam system:

$$Q_{14} = h_{14}A_{14}\ (C_C - C_{14}) \tag{15a}$$

$$= \frac{p_{14}A_{14}}{t_{14}}\ \left[(k_{14}C_{14})^{\frac{1}{2}} - (k_{22}C_{22})^{\frac{1}{2}}\right]\ . \tag{15b}$$

6. Transport through the reheater tubes into the steam system:

$$Q_{15} = h_{15}A_{15}\ (C_C - C_{15}) \tag{16a}$$

$$= \frac{p_{15}A_{15}}{t_{15}}\ \left[(k_{15}C_{15})^{\frac{1}{2}} - (k_{23}C_{23})^{\frac{1}{2}}\right]\ . \tag{16b}$$

7. Removal by sorber as hydrogen:

$$Q_{16} = h_{16}A_{16}\ (C_C - C_{16}) \tag{17a}$$

$$= B_3W_3A_{16}(k_{16}C_{16})^{\frac{1}{2}}\ . \tag{17b}$$

8. Removal by purge as hydrogen:

$$Q_{17} = F_3E_3C_C \ . \tag{18}$$

9. Removal by sorber as HF:

$$Q_{18} = h_{18}A_{18}(C_{CF} - C_{18}) \tag{19a}$$

$$= B_4W_4A_{18}(k_{18}C_{18})^{\frac{1}{2}} \ . \tag{19b}$$

10. Removal by purge as HF:

$$Q_{19} = F_4E_4C_{CF} \ . \tag{20}$$

Since we assume that the hydrogen fluoride does not release hydrogen to diffuse through the metal walls, and that there are no chemical reactions in the secondary system that make the concentrations of hydrogen and hydrogen fluoride interdependent, we write separate material balances for the two species for the distribution of total tritium and hydrogen:

$$R_3 + R_4 = \sum_{i=10}^{17} Q_i \tag{21a}$$

$$R_5 = Q_{18} + Q_{19} \ . \tag{21b}$$

In these equations all the R's and all the Q's have positive or zero values except for Q_{12}, Q_{13}, Q_{14} and Q_{15}, which can have negative values.

C. Steam generator system:

1. Transport through the steam generator tubes into the secondary system:

$$Q_{21} = h_{21}A_{13}(C_{SG} - C_{21}) \tag{22a}$$

$$= \frac{p_{13}A_{13}}{t_{13}}\left[(k_{21}C_{21})^{\frac{1}{2}} - (k_{13}C_{13})^{\frac{1}{2}}\right] \ . \tag{22b}$$

2. Transport through superheater tubes into the secondary system:

$$Q_{22} = h_{22}A_{14}(C_{SS} - C_{22}) \tag{23a}$$

$$= \frac{p_{14}A_{14}}{t_{14}} \left[(k_{22}C_{22})^{\frac{1}{2}} - (k_{14}C_{14})^{\frac{1}{2}} \right] . \tag{23b}$$

3. Transport through the reheater tubes into the secondary system:

$$Q_{23} = h_{23}A_{15}(C_{SR} - C_{23}) \tag{24a}$$

$$= \frac{p_{15}A_{15}}{t_{15}} \left[(k_{23}C_{23})^{\frac{1}{2}} - (k_{15}C_{15})^{\frac{1}{2}} \right] . \tag{24b}$$

In the steam system the values for C_{SG}, C_{SS} and C_{SR} will be given. The steam flows will be so large that the diffusion of hydrogen through the metals should not have much effect on the concentration of hydrogen in the steam. Under these assumptions, we do not require a material balance over the steam system. If hydrogen is added to the feed water as hydrazine or in some other manner to give a specified ratio of hydrogen to H_2O, then this ratio, coupled with the steam tables, can be used to calculate the hydrogen concentrations in the water and steam in the steam-raising equipment. Without addition of hydrogen the concentrations are established by the dissociation of water.

We now need to solve the above equations to obtain values for all the flow rates and concentrations. We carry this out in the following sequence, discussed in more detail in Sec. III.

1. Calculate C_{CF}, C_{18}, Q_{18} and Q_{19} from equations 19a, 19b, 20 and 21b.
2. Assume a value for C_C.
3. Calculate Q_{10}, Q_{11}, Q_{16}, Q_{17} and C_{16} from equations 11a, 11b, 12a, 12b, 17a, 17b and 18.
4. Calculate Q_{13}, Q_{14}, Q_{15}, C_{13}, C_{14} and C_{15} from equations 14a, 14b, 15a, 15b, 16a, 16b, 22a, 22b, 23a, 23b, 24a and 24b, noting that the steam system and the secondary system are coupled by the relationships $Q_{13} = -Q_{21}$, $Q_{14} = -Q_{22}$ and $Q_{15} = -Q_{23}$.

5. Calculate Q_{12} from the material balance, Eq. 21a.

6. Calculate C_F, C_{12} and C_4 from Eqs. 4a, 4b, 13a, 13b, the relationship $Q_4 = -Q_{12}$ and the value of Q_{12} obtained in step 5. These concentrations should all be positive. If any one of them is negative, steps 3 through 6 must be repeated with a larger value of C_C.

7. When positive values have been found for C_F, C_{12} and C_4, calculate Q_1, Q_2, Q_3, Q_5, Q_6, Q_7, Q_8, C_5, C_{FF} and C_7.

8. Calculate R_F from

$$R_F = \sum_{i=1}^{8} Q_i - (R_1 + R_2) \ .$$

If R_F is positive, hydrogen must be added to the primary system in order to maintain a balance. This means that C_F is too large, which in turn means that C_C is too large, and steps 3 through 8 must be repeated with a smaller value of C_C. If R_F is negative, C_C is too small and steps 3 through 8 must be repeated with a larger value of C_C.

When this process has been repeated until the ratio $\left|\frac{R_F}{R_1 + R_2}\right|$ is sufficiently small, the flows and concentrations of hydrogen plus tritium and of hydrogen fluoride plus tritium fluoride have been established throughout the plant and we can proceed with the calculation of the tritium distribution. We ignore the difference in the properties of the two isotopes and assume that they behave identically. Thus, hydrogen and tritium compounds have the same solubilities and diffusivities, and if a hydrogenous compound, such as HF, is added to a mixture of hydrogen and tritium, exchange will occur to give a ratio of tritium to hydrogen that is the same in hydrogen* and the added compound.

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*H_2, HT and T_2.

We now proceed with the calculation of the tritium distribution.

D. Primary system:

1. Transport through walls of hot-leg piping:

$$Q_{31} = \frac{C_{FT}}{C_F} Q_1 \; . \tag{25}$$

2. Transport through walls of cold-leg piping:

$$Q_{32} = \frac{C_{FT}}{C_F} Q_2 \; . \tag{26}$$

3. Transport through wall of reactor vessel and shells of heat exchangers in primary system:

$$Q_{33} = \frac{C_{FT}}{C_F} Q_3 \; . \tag{27}$$

4. Transport through walls of primary heat-exchanger tubes into the secondary system:

$$Q_{34} = h_4 A_4 \; (C_{FT} - C_{34}) \tag{28a}$$

$$= \frac{p_4 A_4}{t_4} \left[\frac{k_4 C_{34}}{(k_4 C_4)^{\frac{1}{2}}} - \frac{k_{12} C_{42}}{(k_{12} C_{12})^{\frac{1}{2}}} \right] \; . \tag{28b}$$

Equations 25 through 27 are straightforward, simply indicating that the amount of tritium flowing with hydrogen is proportional to the fraction of the concentration that is tritium when the flow of both is into a sink with a zero concentration of both. Equation 28a is straightforward, indicating that the flow of tritium from the bulk salt to the wall is proportional to the difference between the concentrations of tritium in the bulk fluid and the wall. Equation 28b, however, requires some additional explanation.

The rate of transport of hydrogen through a metal wall can be expressed as

$$Q = \frac{DA}{t} (C'_I - C'_O) \ ,$$

where D is the diffusivity of hydrogen atoms in the metal, the C's are the concentrations of hydrogen atoms dissolved in the metal at the inner (I) and outer (O) surfaces, t is the metal thickness and A is the surface area. Assuming no interaction of tritium and hydrogen atoms as they diffuse through the metal, the rate of transport of tritium is

$$Q_T = \frac{DA}{t} (C'_{TI} - C'_{TO}) \ .$$

The concentration of hydrogen + tritium atoms in the metal at the surface is

$$C' = SP^{\frac{1}{2}} = S(kC)^{\frac{1}{2}} \ ,$$

where S is a solubility coefficient and P is the partial pressure of hydrogen + tritium and is equal to the product of Henry's law coefficient and the concentration of hydrogen + tritium in the salt at the surface. Assuming that the ratio of tritium to hydrogen + tritium in the metal at the surface is the same as that in the salt at the surface, we can write

$$C'_{TI} = C'_T \frac{C_{TI}}{C_I} = S(k_I C_I)^{\frac{1}{2}} \frac{C_{TI}}{C_I} = S \frac{k_I C_{TI}}{(k_I C_I)^{\frac{1}{2}}}$$

and a similar expression for the outer surface. Then,

$$Q_T = \frac{DSA}{t} \left[\frac{k_I C_{TI}}{(k_I C_I)^{\frac{1}{2}}} - \frac{k_O C_{TO}}{(k_O C_O)^{\frac{1}{2}}} \right] \ ,$$

and by substituting the permeability coefficient, p, for the product, DS, we obtain Eq. 28b. This treatment is necessary here because the net flows of hydrogen and tritium may be in opposite directions. The equations provide a means for taking into account the effect of the mass action laws on the concentrations of tritium in the metal and its transport through the metal.

5. Removal by graphite or other sorber:

$$Q_{35} = \frac{C_{FT}}{C_F} Q_5 \ . \tag{29}$$

6. Removal by purge:

$$Q_{36} = \frac{C_{FT}}{C_F} Q_6 \ . \tag{30}$$

7. Removal by graphite or other sorber as tritium fluoride:

$$Q_{37} = \frac{C_{FT}}{C_F} Q_7 \ . \tag{31}$$

8. Removal by purge as tritium fluoride:

$$Q_{38} = \frac{C_{FT}}{C_F} Q_8 \ . \tag{32}$$

The tritium balance over the primary system is:

$$R_1 = \sum_{i=31}^{38} Q_i \ . \tag{33}$$

E. Secondary system:

1. Hot-leg piping:

$$Q_{40} = \frac{C_{CT}}{C_C} Q_{10} \ . \tag{34}$$

2. Cold-leg piping:

$$Q_{41} = \frac{C_{CT}}{C_C} Q_{11} \quad . \tag{35}$$

3. Transport through primary heat exchanger tube walls into primary system:

$$Q_{42} = h_{12}A_4(C_{CT} - C_{42}) . \tag{36a}$$

$$= \frac{p_4 A_4}{t_4}\left[\frac{k_{12}C_{42}}{(k_{12}C_{12})^{\frac{1}{2}}} - \frac{k_4 C_{34}}{(k_4 C_4)^{\frac{1}{2}}}\right] . \tag{36b}$$

4. Transport through steam generator tube walls into the steam system:

$$Q_{43} = h_{13}A_{13}(C_{CT} - C_{43}) \tag{37a}$$

$$= \frac{p_{13}A_{13}}{t_{13}} \frac{k_{13}C_{43}}{(k_{13}C_{13})^{\frac{1}{2}}} \quad . \tag{37b}$$

Calculations of the tritium distribution are based on the assumption that tritium will exchange so rapidly with the hydrogen in the steam to form tritiated water that the tritium concentration will be effectively zero.

5. Transport through the superheater tubes into the steam system:

$$Q_{44} = h_{14}A_{14}(C_{CT} - C_{44}) \tag{38a}$$

$$= \frac{p_{14}A_{14}}{t_{14}} \frac{k_{14}C_{44}}{(k_{14}C_{14})^{\frac{1}{2}}} \quad . \tag{38b}$$

6. Transport through the reheater tubes into the steam system:

$$Q_{45} = h_{15}A_{15}(C_{CT} - C_{45}) \tag{39a}$$

$$= \frac{p_{15}A_{15}}{t_{15}} \frac{k_{15}C_{45}}{(k_{15}C_{15})^{\frac{1}{2}}} \quad . \tag{39b}$$

7. Removal by sorber as tritium:

$$Q_{46} = \frac{C_{CT}}{C_C} Q_{16} . \qquad (40)$$

8. Removal by purge as tritium:

$$Q_{47} = \frac{C_{CT}}{C_C} Q_{17} . \qquad (41)$$

9. Removal by sorber as tritium fluoride:

$$Q_{48} = \frac{C_{CT}}{C_C} Q_{18} . \qquad (42)$$

10. Removal by purge as tritium fluoride:

$$Q_{49} = \frac{C_{CT}}{C_C} Q_{19} . \qquad (43)$$

The balance over the secondary system is:

$$R_3 = \sum_{i=40}^{49} Q_i . \qquad (44)$$

Since the tritium concentration in the steam system is assumed to be negligible, no equations are needed for the steam system.

To calculate the distribution of tritium, we solve Eqs. 25—44 in the following sequence, discussed in more detail in Section III.

1. Assume a tritium concentration, C_{CT}, in the secondary system and calculate Q_{40}, Q_{41}, Q_{43} through Q_{49} from Eqs. 34, 35, 37a, 37b, 38a, 38b, 39a, 39b, 40, 41, 42 and 43.
2. Calculate Q_{42} from the material balance, Eq. 44.
3. Calculate C_{FT} from Eqs. 28a, 28b, 36a and 36b, the relationship $Q_{34} = -Q_{42}$ and the value of Q_{42} from step 2. If the value of C_{FT} is negative, increase the estimate for C_{CT} and repeat steps 1 through 3. When we have found a positive C_{FT}, we proceed to step 4.

4. Calculate Q_{31}, Q_{32}, Q_{33}, Q_{35}, Q_{36}, Q_{37} and Q_{38} from Eqs. 25—32.

5. Calculate R_F, where

$$R_F = \sum_{i=31}^{38} Q_i - R_1$$

is the term that must be added to the left side of Eq. 33 in order for the equation to balance. If R_F is positive, tritium must be added to the primary system, so C_{FT} and C_{CT} are too large; if R_F is negative, C_{FT} and C_{CT} are too small. Adjust the value of C_{CT} and repeat steps 1 through 5. When $|R_F/R_1|$ is sufficiently small, the calculations are finished.

III. SOLUTION OF EQUATIONS

In the procedure discussed above, we begin with the calculation of C_{CF}, C_{18}, Q_{18} and Q_{19} with Eqs. 19a, 19b and 20, and the material balance, Eq. 21b:

$$Q_{18} = h_{18}A_{18}(C_{CF} - C_{18}) \tag{19a}$$

$$= B_4W_4A_{18}(k_{18}C_{18})^{\frac{1}{2}} \ , \tag{19b}$$

$$Q_{19} = F_4E_4C_{CF} \ , \tag{20}$$

$$R_5 = Q_{18} + Q_{19} \ . \tag{21b}$$

Eq. 19b requires that $Q_{18} \geq 0$ and Eq. 20 requires that $Q_{19} \geq 0$, so if $R_5 = 0$, 21b requires that $Q_{18} = Q_{19} = 0$. If $R_5 > 0$, we combine 21b, 20 and 19a to obtain

$$R_5 - Q_{18} = F_4E_4C_{CF} = R_5 - h_{18}A_{18}(C_{CF} - C_{18}) \ ,$$

or

$$C_{CF} = \frac{R_5+h_{18}A_{18}C_{18}}{F_4E_4+h_{18}A_{18}} \ . \tag{19c}$$

Substituting 19c into 19a, setting the result equal to 19b and collecting terms we obtain

$$\alpha - C_{18} = \beta C_{18}^{\frac{1}{2}} \ , \tag{19d}$$

where we have defined

$$\alpha = \frac{R_5}{F_4E_4} \ ,$$

and

$$\beta = \left[\frac{F_4E_4+h_{18}A_{18}}{F_4E_4}\right]\left[\frac{B_4W_4}{H_{18}}\right]\left[k_{18}\right]^{\frac{1}{2}} \ .$$

Squaring both sides of 19d results in a quadratic equation for C_{18}; since the right-hand side of 19d is positive, we want the root of this quadratic which is less than α. We have

$$C_{18}^2 - (2\alpha+\beta^2)C_{18} + \alpha^2 = 0 ,$$

$$C_{18} = \frac{2\alpha+\beta^2 \pm \sqrt{(2\alpha+\beta^2)^2-4\alpha^2}}{2} .$$

To obtain the root less than α, we want the root with the negative sign. To avoid possible loss of significant figures, we note that the product of the roots is α^2, so that we can write the solution in the form

$$C_{18} = \frac{\alpha^2}{\alpha+\frac{\beta^2}{2}\left(1+\sqrt{1+\frac{4\alpha}{\beta^2}}\right)} . \tag{19e}$$

Then we have

$$Q_{18} = B_4W_4A_{18}(k_{18}C_{18})^{\frac{1}{2}} , \tag{19b}$$

$$C_{CF} = \frac{R_5 + h_{18}A_{18}C_{18}}{F_4E_4 + h_{18}A_{18}} , \tag{19c}$$

and

$$Q_{19} = F_4E_4C_{CF} . \tag{20}$$

With some value for C_C we proceed to the calculation of Q_{10}, Q_{11}, Q_{16}, Q_{17} and C_{16}. Eqs. 11a, 11b, 12a and 12b read

$$Q_{10} = h_{10}A_{10}(C_C - C_{10}) , \tag{11a}$$

$$Q_{10} = \frac{p_{10}A_{10}}{t_{10}}(k_{10}C_{10})^{\frac{1}{2}} , \tag{11b}$$

$$Q_{11} = h_{11}A_{11}(C_C - C_{11}) , \tag{12a}$$

$$Q_{11} = \frac{p_{11}A_{11}}{t_{11}} (k_{11}C_{11})^{\frac{1}{2}} \ . \qquad (12b)$$

These equations (11 and 12) are identical in structure, as are Eqs. 1, 2, 3, 5, 7, 17 and 19. For Eqs. 11 and 12 we define

$$C_1 = C_C, \ \alpha = k_i \left(\frac{p_i}{t_i h_i}\right)^2, \ i = 10, 11 \ ,$$

and Eqs. 11 and 12 then can be written in the form of quadratics in the concentration C_i:

$$C_i^2 - (2C_1 + \alpha)C_i + C_1^2 = 0 \ .$$

From Eqs. 11b and 12b, the flow rates Q_{10} and Q_{11} must be positive, so that the root desired in each case is the smaller one. We have

$$C_i = \frac{C_1^2}{C_1 + \frac{\alpha}{2}\left(1 + \sqrt{1 + \frac{4C_1}{\alpha}}\right)}, \ i = 10, 11 \ ,$$

and

$$Q_i = \frac{p_i A_i}{t_i} (k_i C_i)^{\frac{1}{2}} \ , \ i = 10, 11 \ .$$

By putting

$$C_1 = C_C \ ,$$

$$\alpha = \left(\frac{B_3W_3}{h_{16}}\right)^2 k_{16} \ ,$$

C_{16} can be calculated in the same fashion (Eqs. 17a and 17b) and the flow rates Q_{16} and Q_{17} are

$$Q_{16} = B_3W_3A_{16}(k_{16}C_{16})^{\frac{1}{2}} \ ,$$

$$Q_{17} = F_3E_3C_C \ .$$

We continue with step 4, the calculation of the flow rates Q_{13}, Q_{14} and Q_{15}, and the corresponding concentrations C_{13}, C_{14} and C_{15}, using Eqs. 14a, 14b, 15a, 15b, 16a, 16b, 22a, 22b, 23a, 23b, 24a and 24b. Note that the secondary system and the steam system are coupled by the equations

$$Q_{13} = -Q_{21},\ Q_{14} = -Q_{22} \text{ and } Q_{15} = -Q_{23} .$$

The three equations 14, 15 and 16 all have the same structure and can be written in the form

$$h_K(C_1 - C_K) = \frac{p_K}{t_K}\left[(k_K C_K)^{\frac{1}{2}} - (k_L C_L)^{\frac{1}{2}}\right] , \tag{a}$$

$$h_L(C_L - C_2) = h_K(C_1 - C_K) , \tag{b}$$

where K = 13, 14 and 15, $C_1 = C_C$, L = 21, 22 and 23, and we identify C_2 as C_{SG}, C_{SS} and C_{SR} for K = 13, 14 and 15, respectively. We can solve Eq. b for C_L:

$$C_L = \frac{h_K(C_1 - C_K) + h_L C_2}{h_L} = \frac{h_K}{h_L}(C_1 - C_K) + C_2 . \tag{c}$$

Since C_L must be non-negative, there is a maximum permissible value $C_K^{(max)}$, which is the value such that

$$\frac{h_K}{h_L}\left(C_1 - C_K^{(max)}\right) + C_2 = 0 ,$$

or

$$C_K^{(max)} = C_1 + \frac{h_L}{h_K} C_2 . \tag{d}$$

If we substitute (c) into (a) and rearrange, we have

$$C_K = C_1 + \frac{P_K}{h_K t_K} \left\{ k_L^{\frac{1}{2}} \left[\frac{h_K}{h_L} (C_1 - C_K) + C_2 \right]^{\frac{1}{2}} - \left[k_K C_K \right]^{\frac{1}{2}} \right\}, \tag{e}$$

or, more concisely,

$$C_K = F(C_K) .$$

To locate the solutions (if any) of this equation, we need to examine the behavior of $F(C_K)$ for $0 \leq C_K \leq C_K^{(max)}$. We find that

$$F(0) > 0$$

and

$$F'(C_K) < 0, \; F'(0) = -\infty$$

$$F''(C_K) \geq 0 .$$

The graph of $F(C_K)$ then looks like the curve in Fig. 2.

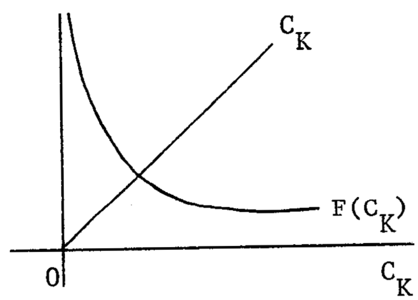

Fig. 2. Sketch of $F(C_K)$ vs C_K.

For there to be a solution between zero and $C_K^{(max)}$, we must have $C_K^{(max)} > F(C_K^{(max)})$ and upon substitution of our expression (d) into $F(C_K)$, we find that this condition is satisfied. We will now examine the function

$$G(C_K) = C_K - F(C_K) .$$

We note that

$$G(0) = -F(0) < 0$$

$$G(C_K^{(max)}) > 0$$

and

$$G'(C_K) = 1 - F'(C_K) > 0 \quad [\text{since } F'(C_K) < 0] .$$

This insures that $G(C_K)$ has one and only one zero in the range $0 \leq C_K \leq C_K^{(max)}$. Since $G''(C_K) = -F''(C_K)$, $G''(C_K) \leq 0$, and the graph of $G(C_K)$ looks like the curve shown in Fig. 3.

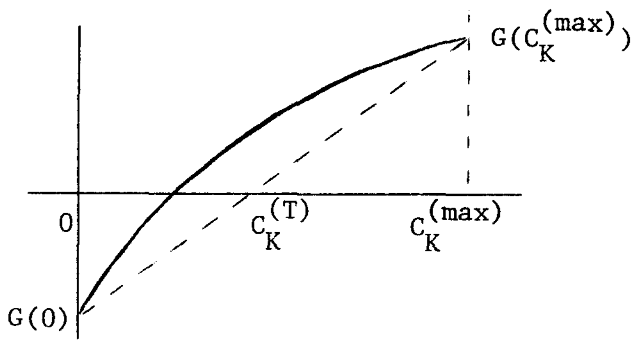

Fig. 3. Sketch of $G(C_K)$ vs C_K

With a suitable $C_K^{(1)}$ we can compute $G_1 = G(C_K^{(1)}) < 0$ (for example, starting with $C_K^{(1)} = 0$) and with a suitable $C_K^{(2)}$, $G_2 = G(C_K^{(2)}) > 0$ ($C_K^{(2)} = C_K^{(max)}$, to start). An approximation to the solution $C_K^{(T)}$, is derived from the inverse linear interpolation:

$$C_K^{(T)} = \frac{G_2 C_K^{(1)} - G_1 C_K^{(2)}}{G_2 - G_1} ,$$

as shown in Fig. 2. A better approximation can be derived with inverse quadratic interpolation:

$$C_K^{(x)} = \frac{(0-G_T)(0-G_2)}{(G_1-G_T)(G_1-G_2)} C_K^{(1)} + \frac{(0-G_1)(0-G_T)}{(G_2-G_1)(G_2-G_T)} C_K^{(2)} + \frac{(0-G_1)(0-G_2)}{(G_T-G_1)(G_T-G_1)} C_K^{(T)} .$$

With $G''(C_K) \leq 0$ as shown and $G'(C_K) > 0$, $G_T = G(C_K^{(T)})$ will be positive and $C_K^{(T)}$ should be larger than the root. If $C_K^{(x)}$ is larger than $C_K^{(T)}$, we replace $C_K^{(2)}$ by $C_K^{(T)}$, G_2 by G_T, and repeat the inverse linear interpolation. If, however, $C_K^{(x)}$ is smaller than $C_K^{(T)}$, we calculate $G_x = G(C_K^{(x)})$; and if this value is negative, we replace $C_K^{(1)}$ by $C_K^{(x)}$, G_1 by G_x, $C_K^{(2)}$ by $C_K^{(T)}$ and G_2 by G_T, and repeat the inverse linear interpolation. If G_x is positive, we replace $C_K^{(2)}$ by $C_K^{(x)}$ and G_2 by G_x and repeat the inverse linear interpolation. We terminate this process when

$$\left| 1 - \frac{C_K^{(T)}}{C_K^{(x)}} \right| < C_{TOL} \; ,$$

or when we have done 50 iterations. The tolerance C_{TOL} is defined in a DATA statement in our program. We have found that the procedure converges in about four iterations for $C_{TOL} = 10^{-5}$ and in about six iterations for $C_{TOL} = 10^{-7}$.

The required flow rates Q_{13}, Q_{21}, Q_{14}, Q_{22}, Q_{15} and Q_{23} can now be computed from

$$Q_i = h_i A_i (C_C - C_i)$$

$$Q_{i+8} = -Q_i , \quad i = 13, 14, 15 \; .$$

The flow rate of hydrogen and tritium through heat exchanger tube walls from the secondary to the primary system, Q_{12}, is

$$Q_{12} = R_3 + R_4 - (Q_{10} + Q_{11} + Q_{13} + Q_{14} + Q_{15} + Q_{16} + Q_{17}) \; ,$$

and from Eq. 13a,

$$C_{12} = C_C - \frac{Q_{12}}{h_{12} A_4} \; .$$

If the value for C_{12} is negative, we have used too small a value for C_C, so we double our previous guess and start over at step 3. If the computed value is positive, we proceed to calculate (Eq. 13b)

$$C_4 = \frac{1}{k_4}\left[(k_{12}C_{12})^{\frac{1}{2}} - \frac{Q_{12}t_4}{p_4A_4}\right]^2 ,$$

and finally,

$$C_F = C_4 - \frac{Q_{12}}{h_4A_4} .$$

If the computed value for C_F is negative, we need a larger value for C_C, so we double our previous guess and return to step 3. If positive, we proceed to step 7, the computation of the remaining flow rates Q_1, Q_2, Q_3, Q_5, Q_6, Q_7 and Q_8 and the concentrations C_5, C_{FF} and C_7.

We can write Eqs. 1, 2 and 3 in the form

$$Q_i = h_iA_i\ (C_F - C_i) = \frac{p_iA_i}{t_i}\ (k_iC_i)^{\frac{1}{2}} ,\ i = 1,\ 2,\ 3,$$

and with

$$\alpha = \left(\frac{p_i}{t_ih_i}\right)^2 k_i$$

the resulting quadratic equations can be solved in the same way as those for C_{10} and C_{11}. Eqs. 5 can be manipulated into the same form with

$$\alpha = \left(\frac{B_1W_1}{h_5}\right)^2 k_5$$

so that we can calculate C_5, and from it

$$Q_5 = B_1W_1A_5\ (k_5C_5)^{\frac{1}{2}} \quad . \tag{5b}$$

Again, Eqs. 7a and 7b can be written as a quadratic for C_7 with

$$\alpha = \left(\frac{B_2W_2}{h_7}\right)^2 k_7$$

so that we can calculate

$$Q_7 = B_2W_2A_7 \; (k_7C_7)^{\frac{1}{2}}$$

$$Q_8 = F_2E_2C_{FF}$$

and

$$R_F = \sum_{i=1}^{8} Q_i - R_1 - R_2$$

where C_{FF} is

$$C_{FF} = \frac{MU}{k_7}\left(k_5C_F\right)^{\frac{1}{2}} \quad . \tag{10}$$

This is the end of the first part of the procedure if R_F is small enough. We test the condition

$$\left|\frac{R_F}{R_1+R_2}\right| < T_{TOL}$$

(where the quantity T_{TOL} is defined in a DATA statement in our program) and if it is satisfied, we proceed to the second part. If not, we adjust C_C in a variety of ways, depending on what information we have accumulated so far. We carry out a preliminary search for two values of C_C which bracket the root, i.e., one for which R_F is negative and the other for which R_F is positive. If this is the first iteration or if both our present and previous values of R_F have the same sign, we multiply C_C by a factor m such that

$$m = 10^{-R_F/(R_1+R_2)}$$

but limited to the range

$$.01 \leq m \leq 100 \quad .$$

When we have bracketed the root, we combine inverse linear and inverse quadratic interpolation in much the same way as we did for the solution of the equations for C_{13}, C_{14} and C_{15}, keeping the root bracketed and attempting to reduce the length of the interval containing the root. When this process has converged, we proceed to the tritium calculation.

With a value for C_{CT}, the concentration of tritium in the secondary salt, we compute

$$Q_{40} = \frac{C_{CT}}{C_C} Q_{10} \tag{34}$$

$$Q_{41} = \frac{C_{CT}}{C_C} Q_{11} \tag{35}$$

and from Eqs. 37a, 37b, 38a, 38b, 39a and 39b we obtain

$$C_{43} = \frac{h_{13}t_{13}(C_{13}/k_{13})^{\frac{1}{2}}/p_{13}}{1+h_{13}t_{13}(C_{13}/k_{13})^{\frac{1}{2}}/p_{13}} C_{CT} \tag{37c}$$

$$Q_{43} = \frac{p_{13}A_{13}}{t_{13}(C_{13}/k_{13})^{\frac{1}{2}}} C_{43} \tag{37b}$$

$$C_{44} = \frac{h_{14}t_{14}(C_{14}/k_{14})^{\frac{1}{2}}/p_{14}}{1+h_{14}t_{14}(C_{14}/k_{14})^{\frac{1}{2}}/p_{14}} C_{CT} \tag{38c}$$

$$Q_{44} = \frac{p_{14}A_{14}}{t_{14}(C_{14}/k_{14})^{\frac{1}{2}}} C_{44} \tag{38b}$$

$$C_{45} = \frac{h_{15}t_{15}(C_{15}/k_{15})^{\frac{1}{2}}/p_{15}}{1+h_{15}t_{15}(C_{15}/k_{15})^{\frac{1}{2}}/p_{15}} C_{CT} \tag{39c}$$

$$Q_{45} = \frac{p_{15}A_{15}}{t_{15}(C_{15}/k_{15})^{\frac{1}{2}}} C_{45} \tag{39b}$$

$$Q_{i+30} = \frac{C_{CT}}{C_C} Q_i, \quad i = 16, 17, 18, 19 \qquad (40\text{-}43)$$

$$Q_{42} = R_3 - Q_{40} - Q_{41} - Q_{43} - Q_{44} - Q_{45} - Q_{46} - Q_{47} - Q_{48} - Q_{49} \qquad (44)$$

and finally

$$C_{42} = C_{CT} - \frac{Q_{42}}{h_{12}A_4} \quad .$$

If this value is negative, we have used too small a value for C_{CT}; in the same way as before, we double C_{CT} and try again, starting at Eq. 34. When we have found a positive C_{42}, we compute

$$C_{34} = \left(\frac{C_4}{k_4}\right)^{\frac{1}{2}} \left[\frac{C_{42}}{(C_{12}/k_{12})^{\frac{1}{2}}} - \frac{t_4 Q_{42}}{p_4 A_4}\right]$$

Again, if C_{34} is negative, we need to double C_{CT} and try again. When we have found a positive C_{34}, we compute

$$C_{FT} = C_{34} - \frac{Q_{42}}{h_4 A_4}$$

and continue with the doubling scheme until C_{42}, C_{34} and C_{FT} are all positive. We can now compute the flow rates

$$Q_{30+i} = \frac{C_{FT}}{C_F} Q_i, \quad i = 1, 2, 3, 5, 6, 7, 8$$

and

$$R_F = \sum_{i=31}^{38} Q_i - R_1 \quad .$$

Our test is now on $\left|R_F/R_1\right|$, and we use the same adjustment and interpolation procedures as for C_C.

IV. NOMENCLATURE

	Reference Value*	Name**
A = surface area, cm^2		A
A_1 = hot leg of primary system (piping and pumps)	6×10^5	
A_2 = cold leg of primary system (piping)	5×10^5	
A_3 = reactor vessel and heat exchanger shells	3.5×10^6	
A_4 = tubes of primary heat exchanger	4.9×10^7	
A_5 = core graphite for sorption of hydrogen	5.2×10^7	
A_6 = --	---	
A_7 = core graphite for sorption of hydrogen fluoride	5.2×10^7	
A_8 = --	---	
A_9 = --	---	
A_{10} = hot leg of secondary system (piping, pumps, half of shells on steam-raising equipment)	1.1×10^7	
A_{11} = cold leg of secondary system (piping, half of shells on steam-raising equipment)	8.8×10^6	
A_{12} = A_4	4.9×10^7	
A_{13} = tubes of steam generators	3.1×10^7	
A_{14} = tubes of superheaters	2.7×10^7	
A_{15} = tubes of reheaters	1.8×10^7	
A_{16} = sorber of hydrogen	0	
A_{17} = --	---	
A_{18} = sorber of hydrogen fluoride	0	

*The reference values are based on the design of a 1000 MWe molten salt breeder reactor plant described in ORNL-4541.

**Acronym used in FORTRAN computer program; if no entry appears, the parameter is not used in the program.

	Reference Value	Name
B = sorption factor, atoms/$cm^2 atm^{1/2}$		B
B_1 = hydrogen + tritium on core graphite	3×10^{21}	
B_2 = hydrogen fluoride on core graphite	3×10^{21}	
B_3 = hydrogen + tritium on sorber in secondary system	1×10^{18}	
B_4 = hydrogen fluoride on sorber in secondary system	1×10^{18}	
C = concentration, atoms/cm^3		
C_F = hydrogen + tritium in bulk of primary salt		CF
C_{FF} = hydrogen + tritium as hydrogen fluoride in bulk of primary salt		CFF
C_{FT} = tritium in bulk of primary salt		CFT
C_C = hydrogen + tritium in bulk of secondary salt		CC
C_{CF} = hydrogen + tritium as hydrogen fluoride in bulk of secondary salt		CCF
C_{CT} = tritium in bulk of secondary salt		CCT
C_{SG} = hydrogen in bulk of water in steam generator (672°K)	2×10^{10}	CSG
C_{SS} = hydrogen in bulk of steam in superheater (783°K)	9×10^{11}	CSS
C_{SR} = hydrogen in bulk of steam in reheater (755°K)	1×10^{11}	CSR
C_1 = hydrogen + tritium in salt at surface of hot leg of primary system		C
C_2 = hydrogen + tritium in salt at surface of cold leg of primary system		
C_3 = hydrogen + tritium in salt at surface of reactor vessel and heat exchanger shells		

	Reference Value	Name
C_4 = hydrogen + tritium in salt at surfaces of heat exchanger tubes in primary system		
C_5 = hydrogen + tritium in salt at surfaces of core graphite in primary system		
C_6 = --		
C_7 = hydrogen fluoride in salt at surfaces of core graphite in primary system		
C_8 = --		
C_9 = --		
C_{10} = hydrogen + tritium in salt at surface of hot leg in secondary system		
C_{11} = hydrogen + tritium in salt at surface of cold leg in secondary system		
C_{12} = hydrogen + tritium in salt at surfaces of heat exchanger tubes in secondary system		
C_{13} = hydrogen + tritium in salt at surfaces of steam generator tubes in secondary system		
C_{14} = hydrogen + tritium in salt at surfaces of superheater tubes in secondary system		
C_{15} = hydrogen + tritium in salt at surfaces of reheater tubes in secondary system		
C_{16} = hydrogen + tritium in salt at surfaces of sorber in secondary system		
C_{17} = --		
C_{18} = hydrogen fluoride in salt at surfaces of sorber in secondary system		
C_{19} = --		

	Reference Value	Name
C_{20} = --		
C_{21} = hydrogen in steam at surfaces of steam generator tubes in steam system		
C_{22} = hydrogen in steam at surfaces of super-heater tubes in steam system		
C_{23} = hydrogen in steam surfaces of reheater tubes in steam system		
C_{24}-C_{33} = --		
C_{34} = tritium in salt at surfaces of heat exchanger tubes in primary system		
C_{35}-C_{41} = --		
C_{42} = tritium in salt at surfaces of heat exchanger tubes in secondary system		
C_{43} = tritium in salt at surfaces of steam generator tubes in secondary system		
C_{44} = tritium in salt at surfaces of super-heater tubes in secondary system		
C_{45} = tritium in salt at surfaces of reheater tubes in secondary system		
E = efficiency		E
E_1 = removal of hydrogen + tritium from purge stream in primary system	5×10^{-1}	
E_2 = removal of hydrogen fluoride from purge stream in primary system	1.7×10^{-2}	
E_3 = removal of hydrogen + tritium from purge stream in secondary system	1.8×10^{-1}	
E_4 = removal of hydrogen fluoride from purge stream in secondary system	1.8×10^{-3}	

	Reference Value	Name
F = flow rate, cm^3/sec		F
F_1 = purge stream for removal of hydrogen + tritium from primary system	3.6×10^5	
F_2 = purge stream for removal of hydrogen fluoride from primary system	3.6×10^5	
F_3 = purge stream for removal of hydrogen + tritium from secondary system	5.0×10^5	
F_4 = purge stream for removal of hydrogen fluoride from secondary system	5.0×10^5	
h = mass transfer coefficient, cm/sec		H
h_1 = hydrogen through primary salt to surfaces of hot leg in primary system	1.6×10^{-2}	
h_2 = hydrogen through primary salt to surfaces of cold leg in primary system	6.0×10^{-3}	
h_3 = hydrogen through primary salt to surfaces of reactor vessel and heat exchanger shells in primary system	9.0×10^{-5}	
h_4 = hydrogen through primary salt to surfaces of heat exchanger tubes in primary system	1.9×10^{-2}	
h_5 = hydrogen through primary salt to surfaces of core graphite in primary system	3.0×10^{-3}	
h_6 = --	---	
h_7 = hydrogen fluoride through primary salt to surfaces of core graphite in primary system	3.0×10^{-3}	
h_8 = --	---	
h_9 = --	---	
h_{10} = hydrogen through secondary salt to surfaces of hot leg in secondary system	7.4×10^{-2}	

	Reference Value	Name
h_{11} = hydrogen through secondary salt to surfaces of cold leg in secondary system	3.4×10^{-2}	
h_{12} = hydrogen through secondary salt to surfaces of tubes in heat exchangers in secondary system	9.7×10^{-2}	
h_{13} = hydrogen through secondary salt to surfaces of tubes of steam generators in secondary system	4.3×10^{-2}	
h_{14} = hydrogen through secondary salt to surfaces of tubes in superheaters in secondary system	4.7×10^{-2}	
h_{15} = hydrogen through secondary salt to surfaces of tubes in reheaters in secondary system	4.0×10^{-2}	
h_{16} = hydrogen through secondary salt to surfaces of sorber in secondary system	8.0×10^{-1}	
h_{17} = --	---	
h_{18} = hydrogen fluoride through secondary salt to surfaces of sorber in secondary system	8.0×10^{-1}	
h_{19} = --	---	
h_{20} = --	---	
h_{21} = hydrogen through water to surfaces of tubes of steam generators in steam system	5.8	
h_{22} = hydrogen through steam to surfaces of tubes of steam generators in steam system	12	
h_{23} = hydrogen through steam to surfaces of tubes of reheaters in steam system	30	

k = Henry's law coefficient, $\frac{(\text{cm}^3\,\text{melt})(\text{atm.})}{\text{atom H}}$ K

$$= 0.83 \times 10^{-24}\left[k' \; \frac{\text{moles } H_2}{(\text{cm}^3\ \text{melt})(\text{atm.})}\right]^{-1}$$

		Reference Value	Name
	$= 1.7 \times 10^{-24} \left[k' \frac{\text{moles HF}}{(\text{cm}^3 \text{ melt})(\text{atm.})} \right]^{-1}$		
k_1	= hydrogen in primary salt in hot leg in primary system (973°K)	1.2×10^{-17}	
k_2	= hydrogen in primary salt in cold leg in primary system (838°K)	2.0×10^{-17}	
k_3	= hydrogen in primary salt in reactor vessel and heat exchanger shells in primary system (908°K)	1.5×10^{-17}	
k_4	= hydrogen in primary salt in heat exchangers in primary system (908°K)	1.5×10^{-17}	
k_5	= hydrogen in primary salt in reactor core in primary system (923°K)	1.4×10^{-17}	
k_6	= --	---	
k_7	= hydrogen fluoride in primary salt in reactor core in primary system (923°K)	1.5×10^{-19}	
k_8	= --	---	
k_9	= --	---	
k_{10}	= hydrogen in secondary salt in hot leg in secondary system (894°K)	3.4×10^{-18}	
k_{11}	= hydrogen in secondary salt in cold leg in secondary system (723°K)	5.0×10^{-18}	
k_{12}	= hydrogen in secondary salt in heat exchangers in secondary system (809°K)	4.0×10^{-18}	
k_{13}	= hydrogen in secondary salt in steam generators in secondary system (783°K)	4.5×10^{-18}	
k_{14}	= hydrogen in secondary salt in superheaters in secondary system (866°K)	3.5×10^{-18}	
k_{15}	= hydrogen in secondary salt in reheaters in secondary system (810°K)	4.0×10^{-18}	

	Reference Value	Name
k_{16} = hydrogen in secondary salt in contact with sorber in secondary system (773°K)	4.4×10^{-18}	
k_{17} = --	---	
k_{18} = hydrogen fluoride in secondary salt in contact with sorber in secondary system (773°K)	1.1×10^{-20}	
k_{19} = --	---	
k_{20} = --	---	
k_{21} = hydrogen in steam in steam generators in steam system (660°K)	4.5×10^{-20}	
k_{22} = hydrogen in steam in superheaters in the steam system (755°K)	5.1×10^{-20}	
k_{23} = hydrogen in steam in reheaters in steam system (714°K)	4.8×10^{-20}	
M = equilibrium quotient for reduction of UF_4 by hydrogen, $atm^{1/2}$, (923°K)	1.12×10^{-6}	M
p = permeability coefficient for hydrogen in metal		P

$$\frac{(\text{atoms H})(\text{mm})}{(\text{sec})(\text{cm}^2)(\text{atm})^{1/2}} = 1.5 \times 10^{16} p' \frac{(\text{cm}^3\ H_2\ \text{STP})(\text{mm})}{(\text{hr})(\text{cm}^2)(\text{atm})^{1/2}}$$

	Reference Value	Name
p_1 = at average temperature of metal in hot leg in primary system (973°K)	2.1×10^{15}	
p_2 = at average temperature of metal in cold leg in primary system (838°K)	6.7×10^{14}	
p_3 = at average temperature of metal in reactor vessel and heat exchanger shells in primary system (873°K)	9.0×10^{14}	
p_4 = at average temperature of metal in tubes in heat exchangers in primary system (873°K)	9.0×10^{14}	

		Reference Value	Name
p_5-p_9	= --	---	
p_{10}	= at average temperature of metal in hot leg in secondary system (893°K)	1.1×10^{15}	
p_{11}	= at average temperature of metal in cold leg in secondary system (723°K)	1.8×10^{14}	
p_{12}	= p_4	9.0×10^{14}	
p_{13}	= at average temperature of tubes in steam generators in secondary system (723°K)	1.8×10^{14}	
p_{14}	= at average temperature of tubes in superheaters in secondary system (838°K)	6.7×10^{14}	
p_{15}	= at average temperature of tubes in reheaters in secondary system (773°K)	3.5×10^{14}	

P = pressure, atm. or other appropriate units

Q = rate of transport, atoms of hydrogen and/or tritium per second — Name: Q

Q_1 = hydrogen + tritium through walls of hot leg in primary system

Q_2 = hydrogen + tritium through walls of cold leg in primary system

Q_3 = hydrogen + tritium through wall of reactor vessel and shells of heat exchangers in primary system

Q_4 = hydrogen + tritium through walls of tubes in heat exchangers from primary system to secondary system

Q_5 = hydrogen + tritium to core graphite in primary system

Q_6 = hydrogen + tritium to purge in primary system

	Reference Value	Name
Q_7 = hydrogen fluoride to core graphite in primary system		
Q_8 = hydrogen fluoride to purge in primary system		
Q_9 = --		
Q_{10} = hydrogen + tritium through walls of hot leg in secondary system		
Q_{11} = hydrogen + tritium through walls of cold leg in secondary system		
Q_{12} = hydrogen + tritium through walls of tubes in heat exchangers from secondary system to primary system = $-Q_4$		
Q_{13} = hydrogen + tritium through walls of the steam generator tubes from the secondary system into the steam system		
Q_{14} = hydrogen + tritium through walls of the superheater tubes from the secondary system into the steam system		
Q_{15} = hydrogen + tritium through walls of the reheater tubes from the secondary system into the steam system		
Q_{16} = hydrogen + tritium to sorber in secondary system		
Q_{17} = hydrogen + tritium to purge in secondary system		
Q_{18} = hydrogen fluoride to sorber in secondary system		
Q_{19} = hydrogen fluoride to purge in secondary system		
Q_{20} = --		
Q_{21} = hydrogen through walls of steam generator tubes from steam system into secondary system = $-Q_{13}$		

	Reference Value	Name

Q_{22} = hydrogen through walls of superheater tubes from steam system into secondary system = $-Q_{14}$

Q_{23} = hydrogen through walls of reheater tubes from steam system into secondary system = $-Q_{15}$

$Q_{24}-Q_{30}$ = --

Q_{31} = tritium through walls of hot leg in primary system

Q_{32} = tritium through walls of cold leg in primary system

Q_{33} = tritium through wall of reactor vessel and shells of heat exchangers in primary system

Q_{34} = tritium through walls of heat exchanger tubes from primary system into secondary system

Q_{35} = tritium to core graphite in primary system

Q_{36} = tritium to purge in primary system

Q_{37} = tritium fluoride to core graphite in primary system

Q_{38} = tritium fluoride to purge in primary system

Q_{39} = --

Q_{40} = tritium through walls of hot leg in secondary system

Q_{41} = tritium through walls of cold leg in secondary system

Q_{42} = tritium through walls of heat exchanger tubes from secondary system into primary system = $-Q_{34}$

		Reference Value	Name
Q_{43}	= tritium through walls of steam generator tubes from secondary system into steam system		
Q_{44}	= tritium through walls of superheater tubes from secondary system into steam system		
Q_{45}	= tritium through walls of reheater tubes from secondary system into steam system		
Q_{46}	= tritium to sorber in secondary system		
Q_{47}	= tritium to purge in secondary system		
Q_{48}	= tritium fluoride to sorber in secondary system		
Q_{49}	= tritium fluoride to purge in secondary system		
R = rate of production or addition, atoms/sec			R
R_1	= tritium in primary system	5.8×10^{17}	
R_2	= hydrogen to primary system	0	
R_3	= tritium in secondary system	0	
R_4	= hydrogen to secondary system	0	
R_5	= hydrogen fluoride to secondary system	0	
R_F	= hydrogen or tritium to primary system in order to obtain overall material balance	---	
T = temperature, °K			
t = wall thickness, mm			T
t_1	= hot leg in primary system	13	
t_2	= cold leg in primary system	13	

		Reference Value	Name
t_3	= reactor vessel and heat exchanger shells in primary system	50	
t_4	= tubes in heat exchangers in primary system	1	
t_5-t_9	= --		
t_{10}	= hot leg in secondary system	13	
t_{11}	= cold leg in secondary system	13	
t_{12}	= t_4		
t_{13}	= tubes in steam generators	2	
t_{14}	= tubes in superheaters	2	
t_{15}	= tubes in reheaters	1	
U	= ratio X_{UF_4}/X_{UF_3}	100	U
W	= replacement rate, fraction/sec		W
W_1	= core graphite or other sorber of hydrogen in primary system	1	
W_2	= core graphite or other sorber of hydrogen fluoride in primary system	1	
W_3	= sorber of hydrogen in secondary system	1	
W_4	= sorber of hydrogen fluoride in secondary system	1	
X	= mole fraction		

V. COMPUTER PROGRAM, INPUT INSTRUCTIONS AND SAMPLE PROBLEM

The FORTRAN-IV program listed in the Appendix was written to provide a flexible and easily used tool for parameter studies. Many of the system parameters listed in Sec. IV have standard or reference values, and we have written the program to allow the user to specify a new value for any parameter, to use the reference value, or to reset a parameter to its reference value. Instructions to the program are in the form of simple commands, followed by numerical values as required.

Output from the program consists of the summary of concentrations, flow rates and fractions shown in Fig. 2, any input commands, and various messages from the program to display the progress of the iterative parts of the calculation.

The three options currently available to the user are

(a) OUTPUT

(b) OUTPUT__ALL_CRBE* — all commands begin in column 1; (the underline indicates a blank space)

(c) OUTPUT__ALL_PRINTER

With choice (a), the summary output is sent to logical unit 20 and all other output is sent to logical unit 6 (the line printer); with choice (b), all output is sent to logical unit 20; and with choice (c), all output is sent to logical unit 6. For choices (a) and (b), appropriate data definition (DD) statements for unit 20 must appear in the user's job control language.

---

*The program was designed to be used from a remote terminal with the Conversational Remote Batch Entry system; hence the use of "CRBE" as a keyword. However, the program in no way depends upon the availability of the CRBE system.

To change various system parameters, the command is

CHANGE__XXX

where XXX is replaced by the appropriate variable name as listed in Sec. IV. If the variable name refers to one of the named concentrations (C_F, C_{FF}, ..., C_{SR}), the next line of input must contain the new parameter value in cols. 1-10. If the variable name refers to any of the subscripted variables in Sec. IV, the next line must contain a starting index, n_1, a stopping index n_2 and the new values for the variables specified by the subscripts n_1 through n_2. A maximum of seven consecutive values is allowed; if there are more than seven, put the subsequent values on subsequent lines. End with a line with a starting index of zero. The following example illustrates the format.

CARD COLUMN

1–6	7–16	17–26	27–36	37
CHANGE	A			
1 3	1.2 +6	1.0 +6	7.0 +6	
13	62. +6			
0				

This will insert new values for A_1, A_2, A_3 and A_{13} of 1.2×10^6, 1.0×10^6, 7.0×10^6 and 62×10^6, respectively. If only one value is to be changed, the second subscript need not appear.

The user can supply *starting estimates* for C_C and C_{CT}, the concentrations of hydrogen plus tritium and tritium in the bulk of the secondary salt, with the "CHANGE" command. If no values are supplied the program will use 1×10^{11} *for* C_C and 1×10^{10} for C_{CT}.

To perform a calculation when all the necessary changes have been made, the command is

RUN

A calculation will then be done with the parameters specified. For subsequent cases, all parameters will have the values present at the end of the preceding calculation; to change the parameters, the user can supply additional "CHANGE" commands. To reset parameters to their reference values, the command is

RESET___XXX

If "XXX" is left blank, all parameters will be reset; if "XXX" is the name of a subscripted variable, all entries with the given name will be reset; and if "XXX" is the name of one of the named concentrations (C_F, C_{FF}, ..., C_{SR}) then just that concentration will be reset. If, for example, after running the case specified by the "CHANGE" command in the example, a user put

RESET___A

then all the A's would be reset to their reference values.

The program will stop when an end-of-file condition is detected on the standard input unit, i.e., when it runs out of data.

The input and output for a sample problem are shown in Figs. 4 and 5. Reference values from Section IV were used in the sample calculation. The results indicate that 30 percent or more of the tritium might reach the steam system in a large power reactor unless special measures are taken to confine the tritium.

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38

```
//XXX1 JØB (nnnnn),'ADDRESS',CLASS=A
// EXEC FØRTHLG,GØSIZE=62K
//LKED.SYSIN DD *
       .
       .
    HEX DECK
       .
       .
/*
//GØ.FT05F001 DD *
ØUTPUT  ALL PRINTER
RUN
CHANGE  A
  1  3 1.2    +6 1.0    +6 7.0    +6
 13    6.2    +7
  0
RUN
ZILCH
/*
//
```

Fig. 4. Sample Problem Input

VALUES IN ARRAY V

NAME A DIMENSION 20 USED 18 STARTS AT 1

1	2	3	4	5
6.00000D 05	5.00000D 05	3.50000D 06	4.90000D 07	5.20000D 07
-1.00000D 00	5.20000D 07	-1.00000D 00	-1.00000D 00	1.10000D 07
8.80000D 06	4.90000D 07	3.10000D 07	2.70000D 07	1.80000D 07
0.0	-1.00000D 00	0.0		

NAME B DIMENSION 5 USED 4 STARTS AT 21

1	2	3	4	5
3.00000D 21	3.00000D 21	1.00000D 18	1.00000D 18	

NAME C DIMENSION 50 USED 45 STARTS AT 26

1	2	3	4	5
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0

NAME CN DIMENSION 10 USED 9 STARTS AT 76

1	2	3	4	5
-1.00000D 00	-1.00000D 00	-1.00000D 00	1.00000D 11	-1.00000D 00
1.00000D 10	2.00000D 10	9.00000D 11	1.00000D 11	

NAME E DIMENSION 5 USED 4 STARTS AT 86

1	2	3	4	5
5.00000D-01	1.70000D-02	1.80000D-01	1.80000D-03	

NAME F DIMENSION 5 USED 4 STARTS AT 91

1	2	3	4	5
3.60000D 05	3.60000D 05	5.00000D 05	5.00000D 05	

NAME H DIMENSION 25 USED 23 STARTS AT 96

1	2	3	4	5
1.60000D-02	6.00000D-03	9.00000D-05	1.90000D-02	3.00000D-03
-1.00000D 00	3.00000D-03	-1.00000D 00	-1.00000D 00	7.40000D-02
3.40000D-02	9.70000D-02	4.30000D-02	4.70000D-02	4.00000D-02
8.00000D-01	-1.00000D 00	8.00000D-01	-1.00000D 00	-1.00000D 00
5.80000D 00	1.20000D 01	3.00000D 01		

Fig. 5A. List of Parameter Values Used in Calculation.

```
VALUES IN ARRAY V

NAME K     DIMENSION  25 USED  23 STARTS AT 121
        1              2              3              4              5

   1.200000D-17   2.000000D-17   1.500000D-17   1.500000D-17   1.400000D-17
  -1.000000D 00   1.500000D-19  -1.000000D 00  -1.000000D 00   3.400000D-18
   5.000000D-18   4.000000D-18   4.500000D-18   3.500000D-18   4.000000D-18
   4.400000D-18  -1.000000D 00   1.100000D-20  -1.000000D 00  -1.000000D 00
   4.500000D-20   5.100000D-20   4.800000D-20

NAME P     DIMENSION  20 USED  15 STARTS AT 146
        1              2              3              4              5

   2.100000D 15   6.700000D 14   9.000000D 14   9.000000D 14  -1.000000D 00
  -1.000000D 00  -1.000000D 00  -1.000000D 00  -1.000000D 00   1.100000D 15
   1.800000D 14   9.000000D 14   1.800000D 14   6.700000D 14   3.500000D 14

NAME R     DIMENSION  10 USED   5 STARTS AT 166
        1              2              3              4              5

   5.800000D 17   0.0            0.0            0.0            0.0

NAME T     DIMENSION  20 USED  15 STARTS AT 176
        1              2              3              4              5

   1.300000D 01   1.300000D 01   5.000000D 01   1.000000D 00  -1.000000D 00
  -1.000000D 00  -1.000000D 00  -1.000000D 00  -1.000000D 00   1.300000D 01
   1.300000D 01   1.000000D 00   2.000000D 00   2.000000D 00   1.000000D 00

NAME W     DIMENSION   5 USED   4 STARTS AT 196
        1              2              3              4              5

   1.000000D 00   1.000000D 00   1.000000D 00   1.000000D 00

NAME M     DIMENSION   1 USED   1 STARTS AT 201
        1              2              3              4              5

   1.120000D-06

NAME U     DIMENSION   1 USED   1 STARTS AT 202
        1              2              3              4              5

   1.000000D 02
```

Fig. 5A. (Continued).

ITERATIVE SOLUTION FOR CC

NCC	CC1	CCL	CCX	RFX	CC2
0				3.47462D 17	1.00000D 11
1	2.52116D 10			-2.91224D 17	
2	2.52116D 10	5.93131D 10		1.62379D 16	1.00000D 11
			5.74238D 10	1.92741D 14	
4	2.52116D 10	5.74025D 10		1.13535D 13	5.74238D 10
			5.74012D 10	1.02747D 08	

ITERATIVE SOLUTION FOR CCT

NCC	CC1	CCL	CCX	RFX	CC2
0	1.00000D 10			-4.71400D 17	
1				4.33784D 16	5.74012D 10

Fig. 5B. Output from Iterative Calculations.

```
OUTPUT SUMMARY

STEAM SYSTEM
    FLOW OF H + T INTO STEAM SYSTEM          1.71072D 17
    FLOW OF T INTO STEAM SYSTEM              1.76310D 17
    FLOW OF H INTO STEAM SYSTEM             -5.23800D 15
    FRACTION OF T INTO STEAM SYSTEM          3.03983D-01

SECONDARY SYSTEM
  FLOWS
    H + T INTO SECONDARY FROM PRIMARY        2.38501D 17
    T INTO SECONDARY FROM PRIMARY            2.39047D 17
    H + T THRU PIPE WALLS INTO CELLS         6.22626D 16
    T THRU PIPE WALLS INTO CELLS             5.79300D 16
  SORPTION BY SINK
    H + T                                    0.0
    T                                        0.0
    HF                                       0.0
    TF                                       0.0
  REMOVAL BY PURGE
    H + T                                    5.16611D 15
    T                                        4.80662D 15
    HF                                       0.0
    TF                                       0.0
  FRACTION OF T
    PASSING THRU PIPE WALLS                  9.98793D-02
    SORBED BY SINK AS T                      0.0
    SORBED BY SINK AS TF                     0.0
    REMOVED BY PURGE AS T                    8.28727D-03
    REMOVED BY PURGE AS TF                   0.0
  CONCENTRATIONS IN SECONDARY SALT
    H + T (CC)                               5.74012D 10
    T (CCT)                                  5.34069D 10
    HF (CCF)                                 0.0


PRIMARY SYSTEM
  FLOWS
    H + T THRU WALLS INTO CELL               3.68436D 15
    T THRU WALLS INTO CELL                   3.67847D 15
  SORPTION BY SINK
    H + T                                    4.45130D 16
    T                                        4.44419D 16
    HF                                       2.32807D 17
    TF                                       2.32435D 17
  REMOVAL BY PURGE
    H + T                                    5.13612D 16
    T                                        5.12791D 16
    HF                                       9.13321D 15
    TF                                       9.11861D 15
  FRACTION OF T
    PASSING THRU WALLS INTO CELL             6.34219D-03
    SORBED BY SINK AS T                      7.66239D-02
    SORBED BY SINK AS TF                     4.00750D-01
    REMOVED BY PURGE AS T                    8.84122D-02
    REMOVED BY PURGE AS TF                   1.57217D-02
  CONCENTRATIONS IN PRIMARY SALT
    H + T (CF)                               2.85340D 11
    T(CFT)                                   2.84884D 11
    HF (CFF)                                 1.49235D 12
```

Fig. 5C. Output Summary.

```
A    ( 1, 3)
   1.200000 06    1.000000 06    7.000000 06
A    (13,13)
   6.200000 07
```

Fig. 5D. Output Produced by "CHANGE" Command.

VALUES IN ARRAY V

NAME A DIMENSION 20 USED 18 STARTS AT 1

1	2	3	4	5
1.20000D 06	1.000000 06	7.000000 06	4.900CCD 07	5.200000 07
-1.C00000 00	5.200000 07	-1.000000 00	-1.000CCD 00	1.100000 07
8.800000 06	4.900000 07	6.200000 07	2.700CCD 07	1.800000 07
0.0	-1.000000 00	0.0		

NAME B DIMENSION 5 USED 4 STARTS AT 21

1	2	3	4	5
3.000000 21	3.000000 21	1.0C000D 18	1.000CCD 18	

NAME C DIMENSION 50 USED 45 STARTS AT 26

1	2	3	4	5
7.944140 07	6.585480 07	1.620350 05	7.732730 10	6.944380-09
0.0	1.622450-05	0.0	0.0	6.136180 08
2.996290 09	2.873180 11	6.774C80 08	1.37958C 10	1.413130 09
4.061490 02	0.0	0.0	0.0	0.0
2.038670 10	9.001530 11	1.000690 11	0.0	0.0
0.0	0.0	0.0	0.0	C.C
0.0	0.0	0.0	2.867830 10	0.0
0.0	0.0	0.0	0.0	0.0
0.0	1.055700 11	3.167720 08	4.74597C 08	1.165100 08

NAME CN DIMENSION 10 USED 9 STARTS AT 76

1	2	3	4	5
3.118030 11	1.560020 12	2.901430 11	5.2842CD 10	0.0
5.435520 10	2.000000 10	9.000000 11	1.000CCC 11	

NAME E DIMENSION 5 USED 4 STARTS AT 86

1	2	3	4	5
5.C0000D-01	1.70000D-02	1.80000D-01	1.800CCD-03	

NAME F DIMENSION 5 USED 4 STARTS AT 91

1	2	3	4	5
3.600000 05	3.600000 05	5.000000 05	5.000000 05	

NAME H DIMENSION 25 USED 23 STARTS AT 96

1	2	3	4	5
1.60000D-02	6.00000D-03	9.00000D-05	1.900CCD-02	3.00000D-03
-1.000000 00	3.00000D-03	-1.0C0000 00	-1.00000C 00	7.40000D-02
3.40C00D-02	9.70000D-02	4.30000D-02	4.700CCD-02	4.C0000D-02
8.00000D-01	-1.000000 C0	8.00000D-01	-1.COCCCD 00	-1.C00000 00
5.800000 00	1.200000 01	3.000000 01		

Fig. 5E. List of Parameter Values Used in Calculation After "CHANGE" Command.

```
VALUES IN ARRAY V

NAME K     DIMENSION  25 USED  23 STARTS AT 121
      1              2              3              4              5

  1.200000D-17   2.000000D-17   1.500000D-17   1.500000D-17   1.400000D-17
 -1.000000D 00   1.500000D-19  -1.000000D 00  -1.000000D 00   3.400000D-18
  5.000000D-18   4.000000D-18   4.500000D-18   3.500000D-18   4.000000D-18
  4.400000D-18  -1.000000D 00   1.100000D-20  -1.000000D 00  -1.000000D 00
  4.500000D-20   5.100000D-20   4.800000D-20

NAME P     DIMENSION  20 USED  15 STARTS AT 146
      1              2              3              4              5

  2.100000D 15   6.700000D 14   9.000000D 14   9.000000D 14  -1.000000D 00
 -1.000000D 00  -1.000000D 00  -1.000000D 00  -1.000000D 00   1.100000D 15
  1.800000D 14   9.000000D 14   1.800000D 14   6.700000D 14   3.500000D 14

NAME R     DIMENSION  10 USED   5 STARTS AT 166
      1              2              3              4              5

  5.800000D 17   0.0            0.0            0.0            0.0

NAME T     DIMENSION  20 USED  15 STARTS AT 176
      1              2              3              4              5

  1.300000D 01   1.300000D 01   5.000000D 01   1.000000D 00  -1.000000D 00
 -1.000000D 00  -1.000000D 00  -1.000000D 00  -1.000000D 00   1.300000D 01
  1.300000D 01   1.000000D 00   2.000000D 00   2.000000D 00   1.000000D 00

NAME W     DIMENSION   5 USED   4 STARTS AT 196
      1              2              3              4              5

  1.000000D 00   1.000000D 00   1.000000D 00   1.000000D 00

NAME M     DIMENSION   1 USED   1 STARTS AT 201
      1              2              3              4              5

  1.120000D-06

NAME U     DIMENSION   1 USED   1 STARTS AT 202
      1              2              3              4              5

  1.000000D 02
```

Fig. 5E. (Continued).

ITERATIVE SOLUTION FOR CC

NCC	CC1	CCL	CCX	RFX	CC2
0				1.44089D 17	5.74012D 10
1	3.24168D 10			-1.33923D 17	
2	3.24168D 10	4.44522D 10		2.91408D 15	5.74012D 10
			4.41906D 10	6.33182D 12	
4	3.24168D 10	4.41900D 10		1.41909D 11	4.41906D 10

ITERATIVE SOLUTION FOR CCT

NCC	CC1	CCL	CCX	RFX	CC2
0				1.74565D 17	5.34069D 10
1	2.67277D 10			-2.02375D 17	

Fig. 5F. Output from Iterative Calculations With New Parameters.

```
OUTPUT SUMMARY

STEAM SYSTEM
    FLOW OF H • T INTO STEAM SYSTEM          1.85851D 17
    FLOW OF T INTO STEAM SYSTEM              1.89989D 17
    FLOW OF H INTO STEAM SYSTEM             -4.13811D 15
    FRACTION OF T INTO STEAM SYSTEM          3.27568D-01

SECONDARY SYSTEM
  FLOWS
    H + T INTO SECONDARY FROM PRIMARY        2.38032D 17
    T INTO SECONDARY FROM PRIMARY            2.38464D 17
    H + T THRU PIPE WALLS INTO CELLS         4.82035D 16
    T THRU PIPE WALLS INTO CELLS             4.47799D 16
  SORPTION BY SINK
    H + T                                    0.0
    T                                        0.0
    HF                                       0.0
    TF                                       0.0
  REMOVAL BY PURGE
    H + T                                    3.97710D 15
    T                                        3.69463D 15
    HF                                       0.0
    TF                                       0.0
  FRACTION OF T
    PASSING THRU PIPE WALLS                  7.72067D-02
    SORBED BY SINK AS T                      0.0
    SORBED BY SINK AS TF                     0.0
    REMOVED BY PURGE AS T                    6.37006D-03
    REMOVED BY PURGE AS TF                   0.0
  CONCENTRATIONS IN SECONDARY SALT
    H • T (CC)                               4.41900D 10
    T (CCT)                                  4.10515D 10
    HF (CCF)                                 0.0


PRIMARY SYSTEM
  FLOWS
    H + T THRU WALLS INTO CELL               7.26328D 15
    T THRU WALLS INTO CELL                   7.25410D 15
  SORPTION BY SINK
    H + T                                    4.38759D 16
    T                                        4.38205D 16
    HF                                       2.31135D 17
    TF                                       2.30843D 17
  REMOVAL BY PURGE
    H + T                                    5.06261D 16
    T                                        5.05621D 16
    HF                                       9.06761D 15
    TF                                       9.05616D 15
  FRACTION OF T
    PASSING THRU WALLS INTO CELL             1.25071D-02
    SORBED BY SINK AS T                      7.55526D-02
    SORBED BY SINK AS TF                     3.98006D-01
    REMOVED BY PURGE AS T                    8.71760D-02
    REMOVED BY PURGE AS TF                   1.56141D-02
  CONCENTRATIONS IN PRIMARY SALT
    H + T (CF)                               2.81256D 11
    T(CFT)                                   2.80901D 11
    HF (CFF)                                 1.48164D 12
```

Fig. 5G. Output Summary (New Parameters).

```
ERROR -  UNRECOGNIZED INPUT
CARD IMAGE IS          1         2         3         4         5         6         7         8
              12345678901234567890123456789012345678901234567890123456789012345678901234567890
              ZILCH
```

Fig. 5H. Response to Unrecognized Command Card.

```
NORMAL STOP - ALL DATA PROCESSED
IHC002I STOP      0
```

Fig. 5I. Normal Ending Message.

APPENDIX

PROGRAM LISTING

```
LEVEL  21.6  (DEC 72)                         OS/360  FORTRAN H                                    DATE  74.304/09.17.44

         COMPILER OPTIONS - NAME=  MAIN,OPT=02,LINECNT=55,SIZE=0000K,
                            SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF
  ISN 0002            IMPLICIT REAL*8 (A-H, O-Z)
  ISN 0003            REAL*8 K,M
  ISN 0004            REAL*4 HALL,HOUT,HCRB,HPRT,HCHA,HRES,HRUN,HBLK,HTEE,CARD
  ISN 0005            DIMENSION A(20), B(5), C(50), CN(10), E(5), F(5), H(25),
                     1 K(25), P(20), R(10), T(20), W(5), CARD(20), VALU(7)
  ISN 0006            DIMENSION S(50)
  ISN 0007            EQUIVALENCE (A(1),V(1)), (B(1),V(21)), (C(1),V(26)),
                     1 (CN(1),V(76)), (E(1),V(86)), (F(1),V(91)),(H(1),V(96)),
                     2 (K(1),V(121)), (P(1),V(146)), (R(1),V(166)), (T(1),V(176)),
                     3 (W(1),V(196)), (M,V(201)), (L,V(202))
  ISN 0008            EQUIVALENCE (CN(1),CF), (CN(2),CFF), (CN(3),CFT), (CN(4),CC),
                     1 (CN(5),CCF), (CN(6),CCT), (CN(7),CSG), (CN(8),CSS), (CN(9),CSR)
  ISN 0009            COMMON/BLK2/IN, IOUT, IPR, KOUT, KPR
  ISN 0010            COMMON /BLK1/ V(250)
  ISN 0011            COMMON/BLK3/ IDIM(20), IUSE(20), NM(20), IBEG(20), NMCN(10),
                     1 NVAR,NCN
  ISN 0012            DATA HALL/4HALL /,HOUT/4HOUTP/,HCRB/4HCRBF/,HPRT/4HPRIN/,
                     1      HCHA/4HCHAN/,HRES/4HRESE/,HRUN/4HRUN /,HBLK/4H    /
  ISN 0013            DATA XCLOG/2.3D0/,HTEE/4HT   /
  ISN 0014            DATA CTOL/1.D-7/, TTOL/1.D-7/
                C
                C        CTOL AND TTOL ARE THE CONVERGENCE TOLERANCES FOR CSOLVE
                C        AND TE RESPECTIVELY.
                C
                C        MAIN PROGRAM FOR CALCULATION OF MSBR TRITIUM FLOW
                C
                C
                C        SET UP REFERENCE VALUES IN WORKING ARRAY V
                C
  ISN 0015            CALL SETREF(HBLK)
                C
                C        READ A CARD AND CHECK FOR INSTRUCTIONS
                C
  ISN 0016        100 READ(IN,1,END=997) CARD
  ISN 0017          1 FORMAT(20A4)
  ISN 0018            IF(CARD(1).NE.HOUT) GO TO 120
                C
                C        SET OUTPUT UNIT NUMBERS
                C
  ISN 0020            IF(CARD(3).NE.HALL) GO TO 115
  ISN 0022            IF(CARD(4).NE.HCRB) GO TO 105
  ISN 0024        104 KOUT=IOUT
  ISN 0025            KPR=IOUT
  ISN 0026            GO TO 100
  ISN 0027        105 IF(CARD(4).EQ.HPRT) GO TO 110
  ISN 0029            WRITE(KOUT,2)
  ISN 0030          2 FORMAT(' OUTPUT NOT SPECIFIED CORRECTLY')
  ISN 0031            WRITE(KOUT,20) (I,I=1,8),CARD
  ISN 0032         20 FORMAT(' CARD IMAGE IS',1X,8(9XI1)/15X,8(10H1234567890)/15X,20A4/
                     1 1X)
  ISN 0033            WRITE(KOUT,21)
  ISN 0034         21 FORMAT(' ALL OUTPUT TO SUMMARY UNIT')
  ISN 0035            GO TO 104
  ISN 0036        110 KOUT=IPR
  ISN 0037        114 KPR=IPR
  ISN 0038            GO TO 100
  ISN 0039        115 KOUT=IOUT
  ISN 0040            GO TO 114
                C
                C        CHECK FOR CHANGES IN WORKING VALUES
                C
  ISN 0041        120 IF(CARD(1).NE.HCHA) GO TO 135
  ISN 0043            CALL MATCH(CARD(3),NM,NVAR,NK)
  ISN 0044            IF(NK.NE.0) GO TO 125
  ISN 0046            CALL MATCH(CARD(3),NMCN,NCN,NC)
  ISN 0047            IF(NC.NE.0) GO TO 121
  ISN 0049            WRITE(KOUT,4)
  ISN 0050          4 FORMAT(' ERROR IN CHANGE SPECIFICATIONS')
  ISN 0051        106 WRITE(KOUT,20) (I,I=1,8),CARD
  ISN 0052            GO TO 100
  ISN 0053        121 READ(IN,7) VALU(1)
  ISN 0054          7 FORMAT(E10.0)
  ISN 0055            J=IBEG(4)+NC-1
  ISN 0056            V(J)=VALU(1)
  ISN 0057            WRITE(KOUT,12) CARD(3),VALU(1)
  ISN 0058         12 FORMAT(1X,A4,1PE14.5)
  ISN 0059            GO TO 100
  ISN 0060        125 READ(IN,3) N1,N2,VALU
  ISN 0061          3 FORMAT(2I3,7E10.0)
  ISN 0062            IF(N1.EQ.0) GO TO 100
  ISN 0064            J=IBEG(NK)-1+N1
  ISN 0065            IF(N2.EQ.0) N2=N1
  ISN 0067            L=1
  ISN 0068            DO 130 N=N1,N2
  ISN 0069            V(J)=VALU(L)
  ISN 0070            L=L+1
  ISN 0071            J=J+1
  ISN 0072        130 CONTINUE
  ISN 0073            NV=N2-N1+1
  ISN 0074            WRITE(KOUT,13) CARD(3),N1,N2,(VALU(L),L=1,NV)
  ISN 0075         13 FORMAT(1X,A4,'(',I2,',',I2,')'/(1X1P5E14.5))
```

```
ISN 0076            GO TO 125
              C
              C          CHECK FOR RESET - PUT REFERENCE VALUES BACK INTO V
              C
ISN 0077        135 IF(CARD(1).NE.HRES) GO TO 150
ISN 0079            IF(CARD(3).NE.HBLK) GO TO 137
ISN 0081        136 CALL SETREF(CARD(3))
ISN 0082            GO TO 100
              C
              C          NAME NOT BLANK - TEST AGAINST NM ARRAY
              C
ISN 0083        137 CALL MATCH(CARD(3),NM,NVAR,NK)
ISN 0084            IF(NK.NE.0) GO TO 136
              C
              C          NO MATCH FOUND IN NM - TRY NMCN
              C
ISN 0086            CALL MATCH(CARD(3),NMCN,NCN,NC)
ISN 0087            IF(NC.NE.0) GO TO 136
ISN 0089            WRITE(KOUT,5)
ISN 0090          5 FORMAT(' ERROR IN RESET SPECIFICATIONS')
ISN 0091            GO TO 106
              C
              C          CHECK FOR PRINT
              C
ISN 0092        150 IF(CARD(1).NE.HPRT) GO TO 155
ISN 0094            IF(CARD(3).NE.HBLK) GO TO 152
ISN 0096        151 CALL LOOK(CARD(3))
ISN 0097            GO TO 100
              C
              C          NAME NOT BLANK - TEST AGAINST NM ARRAY
              C
ISN 0098        152 CALL MATCH(CARD(3),NM,NVAR,NK)
ISN 0099            IF(NK.NE.0) GO TO 151
              C
              C          NO MATCH FOUND IN NM - TRY NMCN
              C
ISN 0101            CALL MATCH(CARD(3),NMCN,NCN,NC)
ISN 0102            IF(NC.NE.0) GO TO 151
ISN 0104            WRITE(KOUT,8)
ISN 0105          8 FORMAT(' ERROR IN PRINT SPECIFICATIONS')
ISN 0106            GO TO 106
ISN 0107        155 IF(CARD(1).EQ.HRUN) GO TO 160
ISN 0109            WRITE(KOUT,6)
ISN 0110          6 FORMAT(' ERROR -  UNRECOGNIZED INPUT')
ISN 0111            GO TO 106
ISN 0112        160 KTRY=1
ISN 0113            ISW=1
ISN 0114            NCC=0
ISN 0115            CC2=0.D0
              C
              C          CHECK FOR FAILURE TO SET CC AND CCT
              C
ISN 0116            IF(CC.LE.0.D0) CC=1.D11
ISN 0118            IF(CCT.LE.0.D0) CCT=1.D10
              C
              C          PRINT WORKING ARRAY V ON LINE PRINTER
              C
ISN 0120            KSAV=KOUT
ISN 0121            KOUT=IPR
ISN 0122            CALL NEWPG
ISN 0123            CALL LOOK(HBLK)
ISN 0124            CALL NEWPG
ISN 0125            KOUT=KSAV
ISN 0126            GO TO 200
              C
              C          GET C(18), CCF, Q(18) AND Q(19)
              C          EQS. 19A,B, 20, 21B
              C
ISN 0127        200 C(18)=0.D0
ISN 0128            CCF=0.D0
ISN 0129            Q(18)=0.D0
ISN 0130            Q(19)=0.D0
ISN 0131            CALL NEWPG
ISN 0132            IF(R(5).EQ.0.D0) GO TO 205
ISN 0134            FE=F(4)*E(4)
ISN 0135            HA=H(18)*A(18)
ISN 0136            FEPH=HA+FE
ISN 0137            BW=R(4)*W(4)
ISN 0138            BESQ=(BW*FEPH/(FE*H(18)))**2*K(18)
ISN 0139            ALFA=R(5)/FE
ISN 0140            C(18)=ALFA**2/(ALFA+.5D0*BESQ*(1.D0+DSQRT(1.D0+4.D0*ALFA/BESQ)))
ISN 0141            Q(18)=BW*A(4)*DSQRT(C(18)*K(18))
ISN 0142            CCF=(R(5)+HA*C(18))/FEPH
ISN 0143            Q(19)=CCF*FE
ISN 0144        205 CONTINUE
              C
              C          BEGIN CALCULATION OF QUANTITIES DEPENDENT ON CC
              C          GET C(10), C(11), Q(10), Q(11)
              C          EQS. 11A,B, 12A,B
              C
ISN 0145        300 NCC=NCC+1
ISN 0146            IF(NCC.LE.50) GO TO 301
ISN 0148            WRITE(KOUT,35) HBLK
```

```
ISN 0149          35 FORMAT(' FAILURE IN SOLUTION FOR CC',A1)
ISN 0150             GO TO 100
ISN 0151         301 DO 305 I=10,11
ISN 0152             ALFA=K(I)*(P(I)/(T(I)*H(I)))**2
ISN 0153             CALL COUAD(CC,ALFA,C(I))
ISN 0154             Q(I)=P(I)*A(I)*DSQRT(K(I)*C(I))/T(I)
ISN 0155         305 CONTINUE
               C
               C        GET C(16), Q(16) - EQS. 17A,B
               C
ISN 0156             BW=B(3)*W(3)
ISN 0157             ALFA=K(16)*(BW/H(16))**2
ISN 0158             CALL COUAD(CC,ALFA,C(16))
ISN 0159             Q(16)=BW*A(16)*DSQRT(K(16)*C(16))
               C
               C        GET C(17) - EQ. 18
               C
ISN 0160             Q(17)=F(3)*E(3)*CC
               C
               C        GET C(13), Q(13), C(14), C(14), C(15), Q(15)
               C        EQS. 14A,B, 22A, 15A,B, 23A, 16A,B, 24A
               C
ISN 0161             IGOCF=0
ISN 0162             CALL CSOLVE(CC,CSG,P(13),T(13),H(13),H(21),K(13),K(21),CTOL,
                    1 IGOCF,C(13),C(21))
ISN 0163             IF(IGOCF.LE.0) GO TO 320
ISN 0165             K1=13
ISN 0166             K2=21
ISN 0167             C2=CSG
ISN 0168         315 WRITE(KOUT,30) K1,K2
ISN 0169          30 FORMAT(' FAILURE IN SOLUTION FOR C(',I2,') AND C(',I2,')')
ISN 0170             IGOCF=-1
ISN 0171             CALL CSOLVE(CC,C2,P(K1),T(K1),H(K1),H(K2),K(K1),K(K2),CTOL,
                    1 IGOCF,C(K1),C(K2))
ISN 0172             GO TO 100
ISN 0173         320 CALL CSOLVE(CC,CSS,P(14),T(14),H(14),H(22),K(14),K(22),CTOL,
                    1 IGOCF,C(14),C(22))
ISN 0174             IF(IGOCF.LE.0) GO TO 325
ISN 0176             K1=14
ISN 0177             K2=22
ISN 0178             C2=CSS
ISN 0179             GO TO 315
ISN 0180         325 CALL CSOLVE(CC,CSR,P(15),T(15),H(15),H(23),K(15),K(23),CTOL,
                    1 IGOCF,C(15),C(23))
ISN 0181             IF(IGOCF.LE.0) GO TO 330
ISN 0183             K1=15
ISN 0184             K2=23
ISN 0185             C2=CSR
ISN 0186             GO TO 315
               C
               C        C(13),Q(21),Q(14),Q(22),Q(15),Q(23)
               C
ISN 0187         330 DO 335 I=13,15
ISN 0188             Q(I)=H(I)*A(I)*(CC-C(I))
ISN 0189             Q(8+I)=-Q(I)
ISN 0190         335 CONTINUE
               C
               C        GET C(12), Q(4) AND C(12) - EQS. 21A, 13A,B
               C
ISN 0191             Q(12)=R(3)+R(4)-Q(10)-Q(11)-Q(13)-Q(14)-Q(15)-Q(16)-Q(17)
ISN 0192             Q(4)=-Q(12)
ISN 0193             C(12)=CC-Q(12)/(H(12)*A(4))
ISN 0194             IF(C(12).GT.0.D0) GO TO 340
ISN 0196             IC=12
ISN 0197             WRITE(KOUT,80) NCC,HBLK,CC,IC,C(IC)
ISN 0198          80 FORMAT(1X,I3,' CC',A1,' =',1PE14.5,' C(',I2,') =',E14.5)
               C
               C        IF C(12) IS NEGATIVE, ADJUST CC AND TRY AGAIN
               C
ISN 0199         336 CC=CC+CC
               C
               C        SEE IF AN UPPER LIMIT (CC2) WAS FOUND.
               C        IF SO, DO NOT EXCEED IT.
               C
ISN 0200             IF(CC2.EQ.0.D0) GO TO 300
ISN 0202             IF(CC.LT.CC2) GO TO 300
ISN 0204             CC=0.5D0*(CC2+0.5D0*CC)
ISN 0205             GO TO 300
               C
               C        GET C(4) AND CF - EQS. 13A,B, 4A,B
               C
ISN 0206         340 C(4)=(DSQRT(K(12)*C(12))-Q(12)*T(4)/(P(4)*A(4)))**2/K(4)
ISN 0207             CF=C(4)-Q(12)/(H(4)*A(4))
ISN 0208             IF(CF.GT.0.D0) GO TO 500
               C
               C        IF CF IS NEGATIVE, ADJUST CC AND TRY AGAIN
               C
ISN 0210             WRITE(KOUT,81) NCC,HBLK,CC,HBLK,CF
ISN 0211          81 FORMAT(1X,I3,' CC',A1,' =',1PE14.5,' CF',A1,' =',E14.5)
ISN 0212             GO TO 336
ISN 0213         500 IF(KTRY.NE.1) GO TO 501
ISN 0215             RF1=0.D0
ISN 0216             RF2=0.D0
```

```
ISN 0217          KTRY=2
ISN 0218          NCC=0
ISN 0219          WRITE(KCUT,50)HBLK
ISN 0220       50 FORMAT(' ITERATIVE SOLUTION FOR CC',A1/1X/
                 1 ' NCC',6X,'CC1',11X,'CCL',11X,'CCX',11X,'RFX',11X,'CC2'/1X)
            C
            C          BEGIN CALCULATION OF QUANTITIES DEPENDENT ON CF
            C          GET C(1), C(2), C(3), Q(1), Q(2), Q(3)
            C          EQS. 1A,B, 2A,B, 3A,B
            C
ISN 0221      501 DO 505 I=1,3
ISN 0222          ALFA=K(I)*(P(I)/(T(I)*H(I)))**2
ISN 0223          CALL CQUAD(CF,ALFA,C(I))
ISN 0224          Q(I)=P(I)*A(I)*DSQRT(K(I)*C(I))/T(I)
ISN 0225      505 CONTINUE
            C
            C          GET C(5), Q(5) -   EQS. 5A,B
            C
ISN 0226          BW=P(1)*W(1)
ISN 0227          ALFA=K(5)*(BW/H(5))**2
ISN 0228          CALL CQUAD(CF,ALFA,C(5))
ISN 0229          Q(5)=BW*A(5)*DSQRT(K(5)*C(5))
            C
            C          GET Q(6) - EQ. 6
            C
ISN 0230          Q(6)=F(1)*E(1)*CF
            C
            C          GET CFF - EQ. 10
            C
ISN 0231          CFF=M*L*DSQRT(K(5)*CF)/K(7)
            C
            C          GET C(7), Q(7) -   EQS. 7A,B
            C
ISN 0232          BW=P(2)*W(2)
ISN 0233          ALFA=K(7)*(BW/H(7))**2
ISN 0234          CALL CQUAD(CFF,ALFA,C(7))
ISN 0235          Q(7)=BW*A(7)*DSQRT(K(7)*C(7))
            C
            C          GET Q(8) - EQ. 8
            C
ISN 0236          Q(8)=F(2)*E(2)*CFF
            C
            C          CALCULATE RF FOR EQ. 9
            C
ISN 0237          RSUM=R(1)+R(2)
ISN 0238          RF=Q(1)+Q(2)+Q(3)+Q(4)+Q(5)+Q(6)+Q(7)+Q(8)-RSUM
ISN 0239          TE=RF/RSUM
            C
            C          TEST CONVERGENCE
            C
ISN 0240          IF(DABS(TE).LT.TTOL) GO TO 700
            C
            C          NOT CONVERGED - CHECK KTRY TO SEE WHAT NEXT
            C
ISN 0242          IF(KTRY.NE.2) GO TO 540
            C
            C          KTRY=2 MEANS PRELIMINARY SEARCH FOR CC1 AND CC2
            C          WHICH BRACKET THE ANSWER
            C
ISN 0244          IF (RF.GT.0.D0) GO TO 510
ISN 0246          CC1=CC
ISN 0247          RF1=RF
ISN 0248          WRITE(KCUT,55) NCC,CC1,RF1
ISN 0249       55 FORMAT(1X,I3,1PE14.5,28X,E14.5)
ISN 0250          GO TO 515
ISN 0251      510 CC2=CC
ISN 0252          RF2=RF
ISN 0253          WRITE(KCUT,56) NCC,RF2,CC2
ISN 0254       56 FORMAT(1X,I3,42X,1P2E14.5)
ISN 0255      515 IF(RF1*RF2) 530,520,516
            C
            C          RF1*RF2 POSITIVE SHOULD NEVER HAPPEN - SOMETHING WRONG
            C
ISN 0256      516 WRITE(KCUT,51) HBLK
ISN 0257       51 FORMAT(' RF1*RF2 POSITIVE - SOMETHING FOULED UP IN CC',A1)
ISN 0258          GO TO 100
            C
            C          STILL LOOKING FOR ONE LIMIT - ADJUST CC AND TRY AGAIN
            C          KEEP ADJUSTMENT FACTOR LESS THAN 100 AND GREATER THAN .01
            C
ISN 0259      520 TEXCLG=TE*XCLCG
ISN 0260          IF(DABS(TEXCLG).GT.4.6D0) TEXCLG=DSIGN(4.6D0,TEXCLG)
ISN 0262          ADJ=DLOG(CC)-TEXCLG
ISN 0263          CC=DEXP(ADJ)
ISN 0264          GO TO 300
            C
            C          RF1*RF2 NEGATIVE - ANSWER BRACKETED
            C
ISN 0265      530 KTRY=3
            C
            C          INVERSE LINEAR INTERPOLATION
            C
ISN 0266      535 CCL=(RF1*CC2 - RF2*CC1)/(RF1-RF2)
```

```
ISN 0267          KTRY=4
ISN 0268          IF(ISW.EQ.2) GO TO 537
ISN 0270          CC=CCL
ISN 0271          GO TO 300
ISN 0272      537 CCT=CCL
ISN 0273          GO TO 705
ISN 0274      540 IF(KTRY.EQ.3) GO TO 535
ISN 0276          IF(KTRY.NE.4) GO TO 555
            C
            C          KTRY=4 MEANS INVERSE LINEAR INTERPOLATION HAS BEEN
            C          COMPLETED AND RF(CCL) CALCULATED
            C
ISN 0278          WRITE(KOUT,52) NCC,CC1,CC,RF,CC2
ISN 0279       52 FORMAT(1X,I3,1P2E14.5,14X,2E14.5)
ISN 0280      542 RFT=RF
            C
            C          INVERSE QUADRATIC INTERPOLATION
            C
ISN 0281          D1=RF1-RFT
ISN 0282          D2=RF2-RFT
ISN 0283          D3=D2-D1
ISN 0284          CCX=CCL*RF1*RF2/(D1*D2)-CC1*RFT*RF2/(D1*D3)+CC2*RF1*RFT/(D2*D3)
ISN 0285          IF(CCX.LT.CC1) GO TO 545
ISN 0287          IF(CCX.GT.CC2) GO TO 545
ISN 0289          KTRY=5
ISN 0290          IF(ISW.EQ.2) GO TO 544
ISN 0292          CC=CCX
ISN 0293          GO TO 300
ISN 0294      544 CCT=CCX
ISN 0295          GO TO 705
ISN 0296      545 IF(RFT.LT.0.D0) GO TO 550
ISN 0298          CC2=CCL
ISN 0299          RF2=RFT
ISN 0300          GO TO 530
ISN 0301      550 CC1=CCL
ISN 0302          RF1=RFT
ISN 0303          GO TO 530
            C
            C          KTRY=5 MEANS INVERSE QUADRATIC INTERPOLATION HAS BEEN
            C          COMPLETED AND RF(CCX) CALCULATED
            C
ISN 0304      555 IF(KTRY.NE.5) GO TO 585
ISN 0306      556 RFX=RF
ISN 0307          WRITE(KOUT,53) CCX,RFX
ISN 0308       53 FORMAT(32X,1P2E14.5)
            C
            C          TEST RFT AND RFX TO SEE WHAT NEW LIMITS ARE
            C
ISN 0309          IF(RFX.GT.0.D0) GO TO 570
ISN 0311          IF(RFT.GT.0.D0) GO TO 565
ISN 0313          IF(DABS(RFX).GT.DABS(RFT)) GO TO 550
ISN 0315      560 CC1=CCX
ISN 0316          RF1=RFX
ISN 0317          GO TO 530
ISN 0318      565 CC2=CCL
ISN 0319          RF2=RFT
ISN 0320          GO TO 560
ISN 0321      570 IF(RFT.LT.0.D0) GO TO 580
ISN 0323          IF(RFX.GT.RFT) GO TO 565
ISN 0325      575 CC2=CCX
ISN 0326          RF2=RFX
ISN 0327          GO TO 530
ISN 0328      580 CC1=CCL
ISN 0329          RF1=RFT
ISN 0330          GO TO 575
ISN 0331      585 WRITE(KOUT,54) KTRY
ISN 0332       54 FORMAT(' KTRY =',I4/' ERROR')
ISN 0333          GO TO 100
            C
            C          CALCULATION OF TRITIUM DISTRIBUTION - CCT SET BY
            C          CHANGE INSTRUCTION
            C
ISN 0334      700 KTRY=1
ISN 0335          ISW=2
ISN 0336          NCCT=0
            C
            C          GET C(40) AND Q(41) - EQS. 34 AND 35
            C
ISN 0337      705 NCCT=NCCT+1
ISN 0338          IF(NCCT.LE.50) GO TO 706
ISN 0340          WRITE(KOUT,35) HTEE
ISN 0341          GO TO 100
ISN 0342      706 RATIO=CCT/CC
ISN 0343          C(40)=RATIO*C(10)
ISN 0344          Q(41)=RATIO*C(11)
ISN 0345          QSUM=C(41)+Q(40)
            C
            C          GET C(43),C(44),C(45),Q(43),C(44),C(45) - EQS. 37A,B, 38A,B, 39A,B
            C
ISN 0346          DO 710 I=43,45
ISN 0347          J=I-30
ISN 0348          TC=T(J)*DSQRT(C(J)/K(J))
ISN 0349          HTCCP=TC*H(J)/P(J)
```

```
ISN 0350          C(I)=CCT*HICOP/(1.D0+HICOP)
ISN 0351          Q(I)=F(J)*A(J)*C(I)/TC
ISN 0352          QSUM=C(I)+CSUM
ISN 0353      710 CONTINUE
            C
            C          GET C(46) THRU Q(49) - EQS. 40 THRU 43
            C
ISN 0354          DO 715 I=46,49
ISN 0355          Q(I)=Q(I-30)*RATIO
ISN 0356          QSUM=C(I)+CSUM
ISN 0357      715 CONTINUE
            C
            C          GET C(42) AND Q(34) - EQ. 44 - MATERIAL BALANCE
            C
ISN 0358          Q(42)=F(3)-CSUM
ISN 0359          Q(34)=-C(42)
            C
            C          GET C(42) -EQ. 36A - CHECK FOR POSITIVE
            C
ISN 0360          C(42)=CCT-C(42)/(H(12)*A(4))
ISN 0361          IF(C(42).GT.0.D0) GO TO 725
ISN 0363          IC=42
ISN 0364      721 WRITE(KOUT,80) NCCT,HTEE,CCT,IC,C(IC)
ISN 0365      720 CCT=CCT+CCT
ISN 0366          GO TO 705
            C
            C          C(42) POSITIVE - GET C(34) - EQ. 28B - CHECK FOR POSITIVE
            C
ISN 0367      725 C(34)=(C(42)/DSQRT(C(12)/K(12))-T(4)*C(42)/(P(4)*A(4)))*DSQRT(C(4)
                 $/K(4))
ISN 0368          IF(C(34).GT.0.D0) GO TO 730
ISN 0370          IC=34
ISN 0371          GO TO 721
            C
            C          C(34) POSITIVE - GET CFT - EQ. 28A - CHECK FOR POSITIVE
            C
ISN 0372      730 CFT=C(34)-C(42)/(H(4)*A(4))
ISN 0373          IF(CFT.GT.0.) GO TO 735
ISN 0375          WRITE(KOUT,81) NCCT,HTEE,CCT,HTEE,CFT
ISN 0376          GO TO 720
            C
            C          CFT, C(34) AND C(42) ALL POSITIVE - CHECK KTRY
            C          FOR NEXT STEP
            C
ISN 0377      735 IF(KTRY.NE.1) GO TO 750
ISN 0379          KTRY=2
ISN 0380          RF1=0.D0
ISN 0381          RF2=0.D0
ISN 0382          NCCT=0
ISN 0383          WRITE(KOUT,50) HTEE
ISN 0384      750 RATIF=CFT/CF
ISN 0385          QTSM=0.D0
ISN 0386          DO 755 I=31,38
ISN 0387          IF(I.EQ.34) GO TO 755
ISN 0389          Q(I)=RATIF*Q(I-30)
ISN 0390      755 QTSM=QTSM+C(I)
ISN 0391          RF=QTSM-R(1)
ISN 0392          TF=RF/R(1)
ISN 0393          IF(DABS(TF).LT.TTOL) GO TO 900
ISN 0395          IF(KTRY.NE.2) GO TO 790
ISN 0397          IF(RF.GT.0.D0) GO TO 760
ISN 0399          CC1=CCT
ISN 0400          RF1=RF
ISN 0401          WRITE(KOUT,55) NCCT,CC1,RF1
ISN 0402          GO TO 765
ISN 0403      760 CC2=CCT
ISN 0404          RF2=RF
ISN 0405          WRITE(KOUT,56) NCCT,RF2,CC2
ISN 0406      765 IF(RF1*RF2) 530,770,766
ISN 0407      766 WRITE(KOUT,51) HTEE
ISN 0408          GO TO 100
            C
            C          STILL LOOKING FOR ONE LIMIT - ADJUST CCT AND TRY AGAIN
            C          KEEP ADJUSTMENT FACTOR LESS THAN 100 AND GREATER THAN .01
            C
ISN 0409      770 TFXCLG=TF*XCLG
ISN 0410          IF(DABS(TFXCLG).GT.4.6D0) TFXCLG=DSIGN(4.6D0,TFXCLG)
ISN 0412          ADJ=DLOG(CCT)-TFXCLG
ISN 0413          CCT=DEXP(ADJ)
ISN 0414          GO TO 705
ISN 0415      790 IF(KTRY.EQ.3) GO TO 535
ISN 0417          IF(KTRY.NE.4) GO TO 795
ISN 0419          WRITE(KOUT,52) NCCT,CC1,CCT,RF,CC2
ISN 0420          GO TO 542
ISN 0421      795 IF(KTRY.NE.5) GO TO 585
ISN 0423          GO TO 556
            C
            C          OUTPUT SECTION
            C          SUMMARY OUTPUT TO UNIT KOUT
            C
ISN 0424      900 CALL NEWPG
ISN 0425          WRITE(KOUT,92)
ISN 0426       92 FORMAT(' OUTPUT SUMMARY'/1X)
```

```
ISN 0427            QHTSS=C(13)+C(14)+Q(15)
ISN 0428            QTSS=C(43)+Q(44)+U(45)
ISN 0429            QHSS=CHTSS-QTSS
ISN 0430            RSUM=1.D0/(R(1)+R(3))
ISN 0431            FRTSS=RSUM*QTSS
ISN 0432            WRITE(KCUT,93) QHTSS,QTSS,CHSS,FRTSS
ISN 0433         93 FORMAT(' STEAM SYSTEM'/5X,'FLCW CF H + T INTO STEAM SYSTEM',
                  1 1PE16.5/5X,'FLOW OF T INTO STEAM SYSTEM',E20.5/5X,'FLCW CF H ',
                  2'INTO STEAM SYSTEM',E20.5/5X,'FRACTION OF T INTC STEAM SYSTEM',
                  3 F16.5/1X)
ISN 0434            QHTPW=C(10)+C(11)
ISN 0435            QTPW=C(40)+C(41)
ISN 0436            FRTPW=CTPW*RSUM
ISN 0437            FTSSK=C(46)*RSUM
ISN 0438            FRTSF=C(48)*RSUM
ISN 0439            FRRPT=C(47)*RSUM
ISN 0440            FRRPF=C(49)*RSUM
ISN 0441            WRITE(KCUT,94) Q(4),Q(34),QHTPW,CTPW,C(16),Q(46),Q(18),C(48),
                  1 Q(17),C(47),C(19),Q(49),FRTPW,FTSSK,FRTSF,FRRPT,FRRPF
ISN 0442            WRITE(KCUT,95) CC,CCT,CCF
ISN 0443         94 FORMAT(' SECCNDARY SYSTEM'/'   FLOWS'/5X,'H + T INTC SECONDARY ',
                  1'FRCM PRIMARY',1PE14.5/5X,'T INTO SECCNDARY FROM PRIMARY',E18.5/
                  2 5X,'H + T THRU PIPE WALLS INTC CELLS',E15.5/5X,'T THRU PIPE ',
                  3'WALLS INTC CELLS',E19.5/'   SCRPTION BY SINK'/5X,'H + T',28X,
                  4 F 14.5/5X,'T',32X,E14.5/5X,'HF',31X,E14.5/5X,'TF',31X,E14.5/
                  5'   REMCVAL BY PURGE'/5X,'H + T',28X,E14.5/5X,'T',32X,E14.5/5X,
                  6'HF',31X,E14.5/5X,'TF',31X,E14.5/'   FRACTION CF T'/5X,'PASSING',
                  7' THRU PIPE WALLS',10X,E14.5/5X,'SCRBED BY SINK AS T',14X,E14.5/
                  8 5X,'SCRBEC BY SINK AS TF',13X,E14.5/5X,'REMOVEC BY PURGE AS T',
                  9 12X,E14.5/5X,'REMOVED BY PURGE AS TF',11X,E14.5)
ISN 0444         95 FORMAT('   CCNCENTRATIONS IN SECCNCARY SALT'/5X,'H + T (CC)',23X,
                  1 1PE14.5/5X,'T (CCT)',26X,E14.5/5X,'HF (CCF)',25X,E14.5/1X/1X)
ISN 0445            QHTW=C(1)+C(2)+Q(3)
ISN 0446            QTW=C(31)+C(32)+Q(33)
ISN 0447            FRTWC=CTW*RSUM
ISN 0448            FTSST=C(35)*RSUM
ISN 0449            FTSSTF=C(37)*RSUM
ISN 0450            FTRPT=C(36)*RSUM
ISN 0451            FTRPTF=C(38)*RSUM
ISN 0452            WRITE(KCUT,96) QHTW,QTW,Q(5),C(35),C(7),Q(37),Q(6),Q(36),Q(8),
                  1 C(38),FRTWC,FTSST,FTSSTF,FTRPT,FTRPTF
ISN 0453            WRITE(KCUT,97) CF,CFT,CFF
ISN 0454         96 FORMAT(' PRIMARY SYSTEM'/'   FLCWS'/5X,'H + T THRU WALLS INTO ',
                  1'CELL',1PE21.5/5X,'T THRU WALLS INTO CELL',11X,E14.5/'   SORPTION
                  2BY SINK'/5X,'H + T',28X,E14.5/5X,'T',32X,E14.5/5X,'HF',31X,E14.5/
                  3 5X,'TF',31X,E14.5/'   REMOVAL BY PURGE'/5X,'H + T',28X,E14.5/5X,
                  4'T',32X,E14.5/5X,'HF',31X,E14.5/5X,'TF',31X,E14.5/'   FRACTION OF
                  5T'/5X,'PASSING THRU WALLS INTC CELL',E19.5/5X,'SORBED BY SINK AS '
                  6,'T',14X,E14.5/5X,'SORBED BY SINK AS TF',13X,E14.5/5X,'REMOVED ',
                  7'BY PURGE AS T',12X,E14.5/5X,'REMOVEC BY PURGE AS TF',11X,E14.5)
ISN 0455         97 FORMAT('   CCNCENTRATIONS IN PRIMARY SALT'/5X,'H + T (CF)',23X,
                  1 1PE14.5/5X,'T(CFT)',27X,E14.5/5X,'HF (CFF)',25X,F14.5)
ISN 0456            CALL NEWPG
ISN 0457            GC TC 100
               C
               C       END CF FILE DETECTED ON INPUT UNIT
               C
ISN 0458        997 CALL NEWPG
ISN 0459            WRITE(KCUT,99)
ISN 0460         99 FORMAT(' NORMAL STOP - ALL CATA PRCCESSEC')
ISN 0461            STOP
ISN 0462            END

*OPTIONS IN EFFECT*     NAME=  MAIN,OPT=02,LINECNT=95,SIZE=0000K,

*OPTIONS IN EFFECT*     SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF

*STATISTICS*     SOURCE STATEMENTS =     461 ,PROGRAM SIZE =    10188

*STATISTICS*  NO  DIAGNOSTICS GENERATED

****** END CF COMPILATION ******                              45K BYTES OF CORE NOT USED
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LEVEL  21.6  (DEC 72)                         OS/360  FORTRAN H                                     DATE  74.304/09.19.05

           COMPILER OPTIONS - NAME=  MAIN,OPT=02,LINECNT=95,SIZE=0000K,
                              SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF
   ISN 0002             BLOCK DATA
   ISN 0003             COMMON /BLK3/ IDIM(20), IUSE(20), NM(20), IBEG(20), NMCN(10),
                       & NVAR, NCN
   ISN 0004             DATA IDIM / 20,5,50,10,5,5,25,25,20,10,20,5,1,1,6*0/
   ISN 0005             DATA IUSE / 18,4,45, 9,4,4,23,23,15, 5,15,4,1,1,6*0/
   ISN 0006             DATA IBEG / 1,21,26,76,86,91,96,121,146,166,176,196,201,202,6*0/
   ISN 0007             DATA NM/4HA    ,4HB    ,4HC    ,4HCN   ,4HE    ,4HF    ,4HH    ,
                       &        4HK    ,4HP    ,4HR    ,4HT    ,4HW    ,4HM    ,4HU    /
   ISN 0008             DATA NVAR, NCN / 14, 9 /
   ISN 0009             DATA NMCN / 4HCF   ,4HCFF ,4HCFT ,4HCC   ,4HCCF ,4HCCT ,4HCSG ,
                       &            4HCSS ,4HCSR ,4H    /
   ISN 0010             COMMON /BLK2/ IN, IOUT, IPR, KOUT, KPR
   ISN 0011             DATA IN, IOUT, IPR /5, 20, 6/
                C
                C          IN   - INPUT UNIT NO.
                C          IOUT - AUXILIARY OUTPUT UNIT NO.
                C          IPR  - LINE PRINTER UNIT NO.
                C
   ISN 0012             END

*OPTIONS IN EFFECT*       NAME=  MAIN,OPT=02,LINECNT=95,SIZE=0000K,

*OPTIONS IN EFFECT*       SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF

*STATISTICS*     SOURCE STATEMENTS =       11 ,PROGRAM SIZE =        8

*STATISTICS*  NO  DIAGNOSTICS GENERATED

****** END OF COMPILATION ******                                      129K BYTES OF CORE NOT USED
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          COMPILER OPTIONS - NAME=  MAIN,OPT=02,LINECNT=55,SIZE=0000K,
                             SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF
  ISN 0002              SUBROUTINE SETREF(NAME)
                C          SETS VARIABLES TO THEIR REFERENCE VALUES. IF NAME IS BLANK,
                C          ALL VARIABLES AS SPECIFIED IN THE ARRAY NM WILL BE SET.
                C          IF NAME IS PRNT, ALL VARIABLES IN THE ARRAY VREF
                C          WILL BE PRINTED.
                C
  ISN 0003              IMPLICIT REAL*8 (A-H,O-Z)
  ISN 0004              REAL*4 VWRD,VW,WORD
  ISN 0005              COMMON/BLK3/ IDIM(20), IUSE(20), NM(20), IBEG(..), NMCN(10),
                       1 NVAR,NCN
  ISN 0006              DIMENSION VREF(250), VO1(155), VO2(75)
  ISN 0007              EQUIVALENCE (VO1(1),VREF(96)), (VO2(1),VREF(176))
                C
                C          VO1 AND VO2 ARE DUMMY ARRAYS USED IN THE INITIALIZATION OF
                C          PARTS OF VREF, THE REFERENCE ARRAY.
                C
  ISN 0008              DATA IBLNK/4H    /,IPRT/4HPRNT/
  ISN 0009              DATA VWRD/4HVREF/, VW/4HV   /
  ISN 0010              COMMON/BLK2/IN, IOUT, IPR, KCLT, KPR
  ISN 0011              COMMON /BLK1/ V(250)
                C
                C          THE COMMENT CARDS INTERSPERSED AMONG THE FOLLOWING
                C          CONTINUATION CARDS CAUSE NO TROUBLE WITH THE ORNL COMPILER.
                C          THIS IS CONTRARY TO THE RULE ON PG. 12, GC28-6515-8,
                C          IBM SYSTEM/360 AND SYSTEM/370 FORTRAN IV LANGUAGE.
                C
  ISN 0012              DATA VREF
                C
                C          REFERENCE VALUES FOR A(I)
                C
                       1/.6D6,.5D6,3.5D6,49.D6,52.D6,-1.D0,52.D6,2*-1.D0 ,11.D6,8.8D6,
                       2 49.D6,31.D6,27.D6,18.D6,0.D0,-1.D0,0.D0,2*-1.D0 ,
                C
                C          REFERENCE VALUES FOR B(I)
                C
                       2 3.D21,3.D21,1.D18,1.D18,-1.D0,
                C
                C          REFERENCE VALUES FOR C(I) ARE ALL ZERO
                C
                       3 45*0.D0 ,5*-1.D0 ,
                C
                C          REFERENCE VALUES FOR CN(I)
                C
                       4 6*-1.D0 ,2.D10,9.D11,1.D11,-1.D0,
                C
                C          REFERENCE VALUES FOR E(I)
                C
                       5 .5D0,.017D0,.18D0,.0018D0,-1.D0,
                C
                C          REFERENCE VALUES FOR F(I)
                C
                       6 3.6D5,3.6D5,5.D5,5.D5,-1.D0/
                C
                C          REFERENCE VALUES FOR H(I)
                C
  ISN 0013              DATA VO1/
                       1 1.6D-2,6.D-3,9.D-5,1.9D-2,3.D-3,-1.D0,3.D-3,2*-1.D0 ,
                       2 7.4D-2,3.4D-2,9.7D-2,4.3D-2,4.7D-2,4.0D-2,.8D0,-1.D0,.8D0,
                       3 2*-1.D0 ,5.8D0,12.D0,30.D0,2*-1.D0 ,
                C
                C          REFERENCE VALUES FOR K(I)
                C
                       4 1.2D-17,2.D-17,1.5D-17,1.5D-17,1.4D-17,-1.D0,1.5D-19,2*-1.D0,
                       53.4D-18,5.D-18,4.D-18,4.5D-18,3.5D-18,4.D-18,4.4D-18,-1.D0,
                       X 1.1D-20,2*-1.D0,4.5D-20,5.1D-20,4.8D-20,2*-1.D0,
                C
                C          REFERENCE VALUES FOR P(I)
                C
                       62.1D15,6.7D14,9.0D14,9.0D14,5*-1.D0,1.1D15,1.8D14,9.0D14,1.8D14,
                       76.7D14,3.5D14,5*-1.D0,
                C
                C          REFERENCE VALUES FOR R(I)
                C
                       8 5.6D17,4*0.D0 ,5*-1.D0 /
                C
                C          REFERENCE VALUES FOR T(I)
                C
  ISN 0014              DATA VO2/
                       1 2*13.D0 ,50.D0,1.D0,5*-1.D0 ,2*13.D0 ,1.D0,2*2.D0 ,1.D0,5*-1.D0,
                C
                C          REFERENCE VALUES FOR W(I)
                C
                       2 4*1.D0 ,-1.D0,
                C
                C          REFERENCE VALUE FOR M
                C
                       31.12D-6,
                C
                C          REFERENCE VALUE FOR U
                C
                       4 1.D2/
```

```
                  C
                  C          CHECK NAME
                  C
ISN 0015                 IF(NAME.EQ.IBLNK) GO TO 102
ISN 0017                 IF(NAME.EQ.IPRT) GO TO 115
                  C
                  C          LOOK FOR MATCH IN NM TABLE
                  C
ISN 0019                 CALL MATCH(NAME,NM,NVAR,NK)
ISN 0020                 IF(NK.NE.0) GO TO 101
                  C
                  C          NO MATCH FOUND - PRINT MESSAGE
                  C
                  C
                  C          CHECK NAME AGAINST CN TABLE
                  C
ISN 0022                 CALL MATCH(NAME,NMCN,NCN,KC)
ISN 0023                 IF(KC.EQ.0) GO TO 300
ISN 0025                 J=IBEG(4)+KC-1
ISN 0026                 V(J)=VREF(J)
ISN 0027                 RETURN
ISN 0028             300 WRITE(KOUT,1) NAME
ISN 0029               1 FORMAT(1X/' NO MATCH FOR ',A4,' IN SETREF - NO CHANGE IN V')
ISN 0030                 RETURN
                  C
                  C          NAME = NM(NK)
                  C
ISN 0031             101 N1=NK
ISN 0032                 N2=NK
ISN 0033                 GO TO 103
ISN 0034             102 N1=1
ISN 0035                 N2=NVAR
ISN 0036             103 DO 110 N=N1,N2
ISN 0037                 IT=IUSE(N)
ISN 0038                 J=IBEG(N)
ISN 0039                 DO 105 I=1,IT
ISN 0040                 V(J)=VREF(J)
ISN 0041             105 J=J+1
ISN 0042             110 CONTINUE
ISN 0043                 RETURN
                  C
                  C          PRINT ALL REFERENCE VALUES
                  C
ISN 0044             115 LINES=50
ISN 0045                 WORD=VWRD
ISN 0046                 DO 130 N=1,NVAR
ISN 0047                 IT=IUSE(N)/5+4
ISN 0048                 IF(LINES+IT.LE.50) GO TO 120
ISN 0050                 CALL NEWPG
ISN 0051                 WRITE(KOUT,2) WORD
ISN 0052               2 FORMAT(' VALUES IN ARRAY ',A4)
ISN 0053                 LINES=0
ISN 0054             120 WRITE(KOUT,3) NM(N),IDIM(N),IUSE(N),IBEG(N),(I,I=1,5)
ISN 0055               3 FORMAT(1X/' NAME ',A4,' DIMENSION',I4,' USED',I4,' STARTS AT'I4/
                        1 7X,4(I1,13X),I1/1X)
ISN 0056                 J1=IBEG(N)
ISN 0057                 I1=J1
ISN 0058                 J2=I1+IUSE(N)-1
ISN 0059                 DO 125 J=J1,J2,5
ISN 0060                 I2=MIN0(I1+4,J2)
ISN 0061                 WRITE(KOUT,4) (VREF(I),I=I1,I2)
ISN 0062               4 FORMAT(1X,1P5E14.5)
ISN 0063                 I1=I2+1
ISN 0064             125 CONTINUE
ISN 0065                 LINES=LINES+IT
ISN 0066             130 CONTINUE
ISN 0067                 RETURN
ISN 0068                 ENTRY LOOK
ISN 0069                 WORD=VW
                  C
                  C          PRINTS VALUES IN V SELECTED BY NAME. IF NAME
                  C          IS BLANK, PRINT ALL.
                  C
                  C          CHECK NAME
                  C
ISN 0070                 IF(NAME.EQ.IBLNK) GO TO 132
                  C
                  C          LOOK FOR MATCH IN TABLE
                  C
ISN 0072                 CALL MATCH(NAME,NM,NVAR,NK)
ISN 0073                 IF(NK.NE.0) GO TO 201
                  C
                  C          CHECK NAME AGAINST CN TABLE
                  C
ISN 0075                 CALL MATCH(NAME,NMCN,NCN,KC)
ISN 0076                 IF(KC.EQ.0) GO TO 301
ISN 0078                 J=IBEG(4)+KC-1
ISN 0079                 WRITE(KOUT,6) NMCN(KC), J, V(J)
ISN 0080               6 FORMAT(1X/1X,A4,' =V(',I3,'), VALUE =',1PE14.5)
ISN 0081                 RETURN
ISN 0082             301 WRITE(KOUT,5) NAME
ISN 0083               5 FORMAT(1X/' NO MATCH FOUND FOR ',A4,' IN LOOK - NO PRINT')
ISN 0084                 RETURN
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   ISN 0085        201 N1=NK
   ISN 0086            N2=NK
   ISN 0087            GO TO 135
   ISN 0088        132 N1=1
   ISN 0089            N2=NVAR
                C
                C         PRINT SELECTED VALUES IN V
                C
   ISN 0090        135 LINES=50
   ISN 0091            DO 150 N=N1,N2
   ISN 0092            IT=IUSE(N)/5+4
   ISN 0093            IF(LINES+IT.LE.50) GO TO 140
   ISN 0095            CALL NEWPG
   ISN 0096            WRITE(KOUT,2) WORD
   ISN 0097            LINES=0
   ISN 0098        140 WRITE(KOUT,3) NM(N),IDIM(N),IUSE(N),IBEG(N),(I,I=1,5)
   ISN 0099            J1=IBEG(N)
   ISN 0100            I1=J1
   ISN 0101            J2=I1+IUSE(N)-1
   ISN 0102            DO 145 J=J1,J2,5
   ISN 0103            I2=MINO(I1+4,J2)
   ISN 0104            WRITE(KOUT,4) (V(I),I=I1,I2)
   ISN 0105            I1=I2+1
   ISN 0106        145 CONTINUE
   ISN 0107            LINES=LINES+IT
   ISN 0108        150 CONTINUE
   ISN 0109            RETURN
   ISN 0110            END

*OPTIONS IN EFFECT*      NAME=  MAIN,OPT=02,LINECNT=55,SIZE=0000K,

*OPTIONS IN EFFECT*      SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF

*STATISTICS*     SOURCE STATEMENTS =      109 ,PROGRAM SIZE =      3996

*STATISTICS*  NO  DIAGNOSTICS GENERATED

****** END OF COMPILATION ******                                 105K BYTES OF CORE NOT USED
```

```
LEVEL  21.6  (DEC 72)                         OS/360  FORTRAN H                                DATE  74.304/09.19.44

          COMPILER OPTIONS - NAME=  MAIN,OPT=02,LINECNT=95,SIZE=0000K,
                             SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF
  ISN 0002            SUBROUTINE CSOLVE(C1,C2,PK,TK,HK,HL,KK,KL,EPS,IGOOF,CK,CL)          CSOL 100
  ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
  ISN 0004            REAL*8 KK, KL
  ISN 0005            TEST=100.D0
  ISN 0006            ASSIGN 95 TO K                                                       CSOL 110
  ISN 0007            HKOHL=HK/HL                                                          CSOL 115
  ISN 0008            PCTH=PK/(TK*HK)                                                      CSOL 122
  ISN 0009            CKMAX=C1+C2/HKOHL
                C                                                                          CSOL 130
                C        CHECK FOR SOLUTION                                                CSOL 131
                C                                                                          CSOL 132
  ISN 0010            CK2=CKMAX                                                            CSOL 133
  ISN 0011            G2=CK2-C1+FOTH*DSQRT(KK*CK2)
  ISN 0012            IF(G2.GT.0.) GO TO 85                                                CSOL 135
  ISN 0014            ASSIGN 130 TO K                                                      CSOL 136
  ISN 0015            PRINT 4                                                              CSOL 137
  ISN 0016          4 FORMAT('1NO SOLUTION')                                               CSOL 138
  ISN 0017            IGOOF=1                                                              CSOL 139
  ISN 0018            GO TO 90                                                             CSOL 140
  ISN 0019         85 IF(IGOOF.GE.0) GO TO 95                                              CSOL 141
                C                                                                          CSOL 142
                C        HEADING FOR DEBUG PRINTOUT                                        CSOL 145
                C                                                                          CSOL 150
  ISN 0021         90 PRINT 1, C1, C2, PK, TK, HK, HL, KK, KL, EPS                         CSOL 155
  ISN 0022          1 FORMAT('1CSOLVE ARGUMENTS'/1H0,6X,'C1',12X,'C2',12X,'PK',12X,'TK',CSOL 160
                    X 12X,
                    1 'HK',12X,'HL',12X,'KK',12X'KL',12X'EPS'/1X,1P9E14.5/'0 IT',6X,     CSOL 161
                    2 'CK1',11X,'CKT',11X,'CX',12X,'CK2',10X,'TEST'/1X)                  CSOL 162
  ISN 0023            GO TO K, (95,130)                                                    CSOL 163
                C                                                                          CSOL 165
                C        START ITERATIONS FOR CK                                           CSOL 170
                C                                                                          CSOL 175
  ISN 0024         95 CK1=0.                                                               CSOL 176
  ISN 0025            CKOLD=CK1
  ISN 0026            CL1=KL*(HKOHL*C1+C2)
  ISN 0027            G1=-(C1+PCTH*DSQRT(CL1))
  ISN 0028            DO 115 IT=1,50                                                       CSOL 180
                C
                C        INVERSE LINEAR INTERPOLATION AND CHECK FOR CONVERGENCE
                C
  ISN 0029            CKT=(CK1*G2-CK2*G1)/(G2-G1)                                          CSOL 182
  ISN 0030            IF(DABS(CKOLD/CKT-1.D0).LT.EPS) GO TO 120                            CSOL 183
                C
                C        IF NOT CONVERGED, TRY INVERSE QUADRATIC INTERPOLATION
                C
  ISN 0032            CLT=KL*(HKOHL*(C1-CKT)+C2)
  ISN 0033            FF=C1+PCTH*(DSQRT(CLT)-DSQRT(KK*CKT))
  ISN 0034            G=CKT-FF                                                             CSOL 192
  ISN 0035            DG1=G-G1                                                             CSOL 193
  ISN 0036            DG2=G-G2                                                             CSOL 194
  ISN 0037            DG3=DG2-DG1                                                          CSOL 195
  ISN 0038            CX=-G*G2*CK1/(DG3*DG1)+G1*G2*CKT/(DG1*DG2)+G1*G*CK2/(DG3*DG2)        CSOL 196
  ISN 0039            IF(IGOOF.GE.0) GO TO 200                                             CSOL 240
                C                                                                          CSOL 245
                C        DEBUG PRINTOUT                                                    CSOL 250
                C                                                                          CSOL 255
  ISN 0041            PRINT 2,IT,CK1,CKT,CX,CK2,TEST
  ISN 0042          2 FORMAT(1XI3,1P5E14.5)
  ISN 0043        200 IF(CX.LE.CK1) GO TO 102                                              CSOL 197
  ISN 0045            IF(CX.GE.CKT) GO TO 102                                              CSOL 198
  ISN 0047            TEST=DABS(CKOLD/CX-1.D0)
  ISN 0048            IF(TEST.GT.EPS) GO TO 201
  ISN 0050            CKT=CX
  ISN 0051            GO TO 120
  ISN 0052        201 CLX=KL*(HKOHL*(C1-CX)+C2)
  ISN 0053            FX=C1+PCTH*(DSQRT(CLX)-DSQRT(KK*CX))
  ISN 0054            GX=CX-FX                                                             CSOL 201
  ISN 0055            CKOLD=CX
  ISN 0056            IF(GX.LT.0.) GO TO 101                                               CSOL 202
  ISN 0058            CK2=CX                                                               CSOL 203
  ISN 0059            G2=GX                                                                CSOL 204
  ISN 0060            GO TO 115
  ISN 0061        101 CK1=CX                                                               CSOL 206
  ISN 0062            G1=GX                                                                CSOL 207
  ISN 0063            GO TO 105                                                            CSOL 208
  ISN 0064        102 TEST=DABS(CKOLD/CKT-1.D0)                                            CSOL 225
  ISN 0065            CKOLD = CKT                                                          CSOL 226
  ISN 0066            IF(TEST.LE.EPS) GO TO 120                                            CSOL 227
  ISN 0068            IF (G .EQ. 0.D0) GO TO 120                                           CSOL 230
  ISN 0070            IF(G.GT.0.) GO TO 105                                                CSOL 231
  ISN 0072            G1=G                                                                 CSOL 232
  ISN 0073            CK1=CKT                                                              CSOL 233
  ISN 0074            GO TO 115
  ISN 0075        105 G2=G                                                                 CSOL 235
  ISN 0076            CK2=CKT                                                              CSOL 236
  ISN 0077        115 CONTINUE
                C                                                                          CSOL 275
                C        PRINT NON-CONVERGENCE ALARM                                       CSOL 280
                C                                                                          CSOL 285
  ISN 0078            PRINT 3                                                              CSOL 290
  ISN 0079          3 FORMAT('0 CSOLVE UNABLE TO FIND ROOT')                               CSOL 295
```

```
ISN 0080          IGOCF=MAXO(1,IGOOF+1)                       CSOL 300
ISN 0081          RETURN                                      CSOL 305
ISN 0082      120 CK=CKT                                      CSOL 310
ISN 0083          CL=FKCHL*(CL-CK)+C2
ISN 0084      130 RETURN                                      CSOL 320
ISN 0085          END                                         CSOL 325

*OPTIONS IN EFFECT*     NAME=  MAIN,OPT=02,LINECNT=55,SIZE=0000K,

*OPTIONS IN EFFECT*     SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF

*STATISTICS*     SOURCE STATEMENTS =      84 ,PROGRAM SIZE =      2024

*STATISTICS*  NO  DIAGNOSTICS GENERATED

****** END OF COMPILATION ******                         121K BYTES OF CORE NOT USED
```

```
LEVEL  21.6  (DEC 72)                    OS/360  FORTRAN H                                DATE  74.304/09.20.10

        COMPILER OPTIONS - NAME=  MAIN,OPT=02,LINECNT=55,SIZE=0000K,
                           SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF
  ISN 0002              SUBROUTINE NEWPG
                 C
                 C         IF THE SUMMARY OUTPUT UNIT (KOUT) IS THE LINE PRINTER (IPR),
                 C         EJECT TO A NEW PAGE. IF NOT, PRINT 5 BLANK LINES.
                 C
  ISN 0003              COMMON /BLK2/ IN, IOUT, IPR, KOUT, KPR
  ISN 0004              IF(KOUT.EQ.IPR) GO TO 100
  ISN 0006              WRITE(KOUT,1)
  ISN 0007            1 FORMAT(1X/1X/1X/1X/1X)
  ISN 0008              RETURN
  ISN 0009          100 WRITE(KOUT,2)
  ISN 0010            2 FORMAT(1H1)
  ISN 0011              RETURN
  ISN 0012              END

*OPTIONS IN EFFECT*      NAME=  MAIN,OPT=02,LINECNT=55,SIZE=0000K,

*OPTIONS IN EFFECT*      SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF

*STATISTICS*     SOURCE STATEMENTS =       11 ,PROGRAM SIZE =       260

*STATISTICS*  NO  DIAGNOSTICS GENERATED

****** END OF COMPILATION ******                                  133K BYTES OF CORE NOT USED
```

```
LEVEL  21.6  (DEC 72)                    OS/360  FORTRAN H                                DATE  74.304/09.20.25

        COMPILER OPTIONS - NAME=  MAIN,OPT=02,LINECNT=55,SIZE=0000K,
                           SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF
  ISN 0002              SUBROUTINE CQUAD(C1,ALFA,CK)
                 C
                 C         SOLVES THE QUADRATIC EQUATION
                 C
                 C         CK**2 - (2*C1 + ALFA)*CK + C1**2 = 0
                 C
                 C         FOR THE ROOT CK WHICH IS LESS THAN C1/KK.
                 C
  ISN 0003              IMPLICIT REAL*8 (A-H,O-Z)
  ISN 0004              REAL*8 KK
  ISN 0005              T=C1/KK
  ISN 0006              CK=C1**2/(C1+.5*ALFA*(1.+DSQRT(4.*C1/ALFA+1.)))
  ISN 0007              RETURN
  ISN 0008              END

*OPTIONS IN EFFECT*      NAME=  MAIN,OPT=02,LINECNT=55,SIZE=0000K,

*OPTIONS IN EFFECT*      SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF

*STATISTICS*     SOURCE STATEMENTS =        7 ,PROGRAM SIZE =       444

*STATISTICS*  NO  DIAGNOSTICS GENERATED

****** END OF COMPILATION ******                                  133K BYTES OF CORE NOT USED
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LEVEL  21.6  (DEC 72)                    OS/360  FORTRAN H                                DATE  74.304/09.20.38

        COMPILER OPTIONS - NAME=  MAIN,OPT=02,LINECNT=55,SIZE=0000K,
                           SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF
  ISN 0002              SUBROUTINE MATCH (NAME, NTAB, NN, NMAT)
                 C
                 C         SEARCHES THE ARRAY NTAB WITH NN ITEMS FOR THE FIRST
                 C         OCCURRENCE OF NAME. IF NAME IS NOT FOUND IN NTAB, NMAT
                 C         IS RETURNED WITH THE VALUE ZERO.
                 C
  ISN 0003              DIMENSION NTAB (10)
  ISN 0004              NMAT = 0
  ISN 0005              DO 100 N=1,NN
  ISN 0006              IF (ICOMPA(NAME, NTAB(N), 4) .NE. 0) GO TO 100
  ISN 0008              NMAT = N
  ISN 0009              RETURN
  ISN 0010          100 CONTINUE
  ISN 0011              RETURN
  ISN 0012              END

*OPTIONS IN EFFECT*      NAME=  MAIN,OPT=02,LINECNT=55,SIZE=0000K,

*OPTIONS IN EFFECT*      SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF

*STATISTICS*     SOURCE STATEMENTS =       11 ,PROGRAM SIZE =       398

*STATISTICS*  NO  DIAGNOSTICS GENERATED

****** END OF COMPILATION ******                                  133K BYTES OF CORE NOT USED

*STATISTICS*  NO  DIAGNOSTICS THIS STEP
```

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