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Improved Real Gas Routines for Sandia's NASA Ames Flow Field Program

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IMPROVED REAL GAS ROUTINES FOR SANDIA'S NASA AMES FLOW FIELD PROGRAM

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ABSTRACT

The real gas subroutines in Sandia's version of the NASA Ames flow field code have been extensively revised. Using these modifications the required computer run time for a difficult high Mach number case has been reduced from 1330 seconds to 151 seconds.

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IMPROVED REAL GAS ROUTINES FOR SANDIA'S NASA AMES FLOW FIELD PROGRAM

INTRODUCTION

Sandia's version of the NASA Ames flow field code continues to be used extensively for calculating inviscid gas flow fields along bodies at zero angle of attack. This code in its original form requires extremely large amounts of computer time when calculating with the real equilibrium gas model. Over thirteen hundred seconds of CDC 6600 computer time are required to calculate the flow over a blunted 6° cone for a length of 60 nose radii when $M_{\infty} = 22$ and the altitude, h, is 30 km. This difficult case requires only 24 seconds using an ideal gas model. A less difficult case for the same geometry and using the real gas model for $M_{\infty} = 8$ and h = 0.3 km requires 530 seconds.

With a moderate amount of modifying subroutines RGAS, SERCH and ISENC these same real gas cases can now be computed in 152 seconds and 109 seconds, respectively. The modified code is 5 to 8 times faster than the original code. The time of computation for the original code was strongly dependent on the size of the compressibility factor Z in the equation of state ($p = Z\rho RT$). Some of these calculations have Z larger than 3 when total isentropic properties are being calculated. Ideal gas equations are used as a first approximation to the equilibrium gas solution. The real solution is then obtained using an iterative procedure. The ideal gas equations are not accurate for large Z, thus many iterations must be completed to obtain satisfactory real gas values. In the modified code, the methods used to iterate have been greatly improved.

This report discusses the function of the three subroutines listed above and outlines the recommended changes that must be incorporated into the original code to obtain the reduction in computing time described above.

SUBROUTINE RGAS

The function of the RGAS subroutine is to supply thermodynamic state properties for a gas in chemical equilibrium. Given two state properties the remaining properties

are calculated using the spline fit coefficients which are stored on Tape 9 (hereafter identified as RGAS data or RGAS Tables). If pressure and density are provided, the look up procedure is direct. If pressure and entropy are provided, the look up procedure is iterative. In this latter case the pressure and entropy are used to estimate density which in turn is used with pressure to determine entropy from the tables. This entropy is then compared with the given entropy. The density is incremented and an iteration procedure is followed until the given and calculated values of entropy agree satisfactorily. The final density and given pressure are then used to determine the remaining state properties; enthalpy, temperature, and sonic velocity.

Due to the general use of the RGAS subroutine in this program, a sample problem, a detailed outline and a FORTRAN listing are given in Appendix A, B and C. Prior to studying these Appendices it is important to understand how the spline fit data (Tape 9) is stored, retrieved and used. An outline of this concept follows.

Groups of spline fit coefficients for the four variables and their associated indexing parameters can be thought of as being contained in boxes. There are eleven boxes which are indexed by powers of density.

$R = \log \frac{\rho}{\rho_o} = -7$	$\log \frac{\rho}{\rho_o} = -6$		$\log \frac{\rho}{\rho_o} = 3$
Spline fit coefficients for sonic velocity, enthalpy, temperature, and entropy.	Spline fit coefficients for sonic velocity, enthalpy, temperature, and entropy.	etc.	Spline fit coefficients for sonic velocity, enthalpy, temperature, and entropy.

Sketch 1. Groups of Spline Coefficients

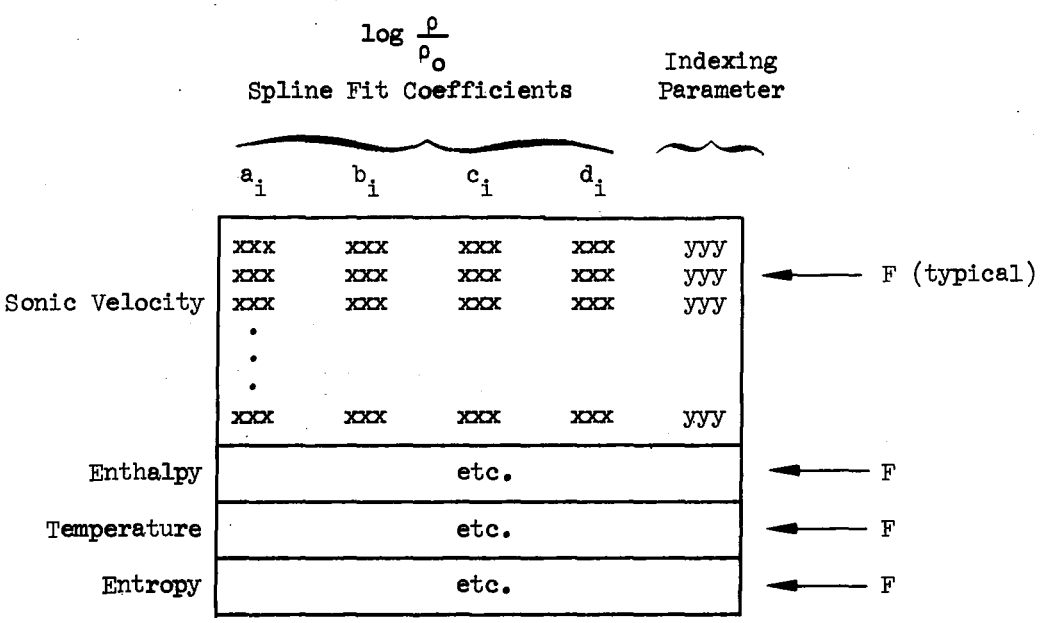
The process of obtaining real gas thermodynamic state properties for a given pressure and density using the information in these boxes can be divided into three general steps.

Step 1

Step one is to locate the two storage boxes that contain coefficients for the densities which bracket the given density. We are now interested only in these two boxes.

Step 2

Both of these boxes contain a complete range of coefficients for the four state variables. In order to isolate the sets of coefficients which are the most closely associated with the given pressure and density, a quantity F is calculated. F is a function of pressure, density and several constants, Figure 1. For each of the four state properties the indexing parameters (see Sketch 2) are searched to find the one that is closest to, but smaller than F.



Sketch 2. Details of Any One of the Boxes Shown in Sketch 1.

These four sets of spline fit coefficients and F are then used to calculate the state properties as follows.

$$Y = a_i + b_i F + c_i F^2 + d_i F^3$$

$$\text{where } Y = \begin{cases} \text{Sonic Velocity} & i = 1 \\ \text{Enthalpy} & i = 2 \\ \text{Temperature} & i = 3 \\ \text{Entropy} & i = 4 \end{cases}$$

and a_i, b_i, c_i and d_i are the spline fit coefficients for the cubic spline.

Step 3

Two values, one from each of the two boxes, have been obtained for each of the four state properties. The final values of the real gas thermodynamic state properties are obtained by interpolating between these boxes.

Several modifications have been made to RGAS. The logic flow has been revised. It is more readable and several of the multiple recalculations of branching variables have been eliminated. Originally numerous calls were made to SERCH for the polynomial coefficient values for F equal zero. Since these values never change, the revised program obtains these values once and stores them in an array for retrieval when needed.

The most significant improvement to RGAS is the reduction in the number of iterations of density when the input is pressure and entropy. This is accomplished by starting the iteration with the density obtained at the previous mesh point along the characteristic line.

SUBROUTINE SERCH

This subroutine searches the arrays filled from the RGAS tape to find the coefficients which correspond with the index F calculated in subroutine RGAS. The original technique, which is valid for data in random order, has been modified to take advantage of the fact that the tables are stored in monotonic order. The original Do Loop required searching through all data points. The revised program, lines 5-8

of Appendix D, uses the monotonic order to exit from the loop immediately after passing the desired value. This Do Loop has been shortened. It now fits "IN STACK"* which saves computer time.

The second time saving improvement consists of replacing the parameter list with a common block. In addition the coding now brackets the midpoint (NER) upon initially entering the subroutine. Consequently, no more than half of the table needs to be examined for each entry into SERCH. The most significant improvement is obtained with the first two revisions.

The third statement of the subroutine sets NOUT equal to 70,000. This is done in order to help debug the program in the event that the subroutine is called with a value of F less than the first position in the RGAS Table (zero for air). In case of this event the program is returned to subroutine RGAS and the calculations fail with a mode one type error on the CDC 6600.

SUBROUTINE ISENC

Subroutine ISENC contains an iteration scheme which is used to obtain state properties at point 2 given entropy (S) at points 1 and 2 and enthalpy (H) at point 1. Points 1 and 2 are adjoining points along a characteristic line. Since RGAS will not use S and H directly the pressure is approximated using an ideal gas equation. P and S are then used in RGAS to obtain the remaining state properties. Next an iteration procedure is used on pressure until the enthalpy calculated in RGAS agrees within a given tolerance to the given enthalpy.

The original subroutine is excessively time consuming; particularly when total isentropic state properties being calculated are quite different from ideal gas approximations. In these cases the ideal gas equations which are used for first

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*Computer programmed instructions are stored in an instruction stack capable of holding eight 60-bit words. Instructions for inner "Do Loops" which can be contained within eight words fit "IN STACK" and are the fastest executing loops.

approximations are not accurate for real equilibrium gas, consequently many iterations must be performed.

In order to describe the improvements made to this program an outline of the original scheme will be given followed by an outline of the modifications made.

Original Subroutine Outline

1. Entropy and enthalpy are known.
2. Pressure (P) is estimated using pressure and Mach number at point 1 and the ideal gas equation.
3. Subroutine RGAS is called with P and S to get remaining state properties.
4. The H from RGAS is compared with given H. If not within given tolerance, P is improved as outlined below.
5. $P_{initial}$ is decreased by a factor ZROOT = 0.97 (Figure 2). Steps 3 and 4 are redone. Checks to see if P was changed in proper direction.
6. If change was in right direction and not too large (doesn't overshoot answer), another increment is taken ($P_{initial}$ x 0.97 x 0.97).
7. If change is in wrong direction, $P_{initial}$ is multiplied by ZROOT = 1.03 (Figure 3). The process of using RGAS to obtain remaining state properties is repeated.
8. New P values are obtained using $P_{initial}$ x $ZROOT^n$ until given H is passed.
9. When answer is bracketed between steps n and n + 1, the properties at the intermediate 1/3 intervals are calculated.
10. Using the four points obtained in Step 9 an interpolation scheme is used in subroutine INTER to calculate the final pressure. RGAS is then used to obtain the final state properties.

Improvements Made to Subroutine ISENC

In situations where the real gas answer differs appreciably from the initial ideal gas estimate the above technique consumes computer time excessively. In some

extreme cases the P had to be incremented in the order of 10^2 times by the factor (ZROOT = 0.97 or ZROOT = 1.03) before the convergence criterion was met. Consequently, the subroutine ISENC has been rewritten to change the convergence technique as follows. Step 1 through 7 given above remain the same. Step 8 is the same the first time through the subroutine. At this point the program stores the final n so that the next time the subroutine is used for a similar type calculation the stored value of n can be used to "jump" (n-3) intermediate steps. See Figure 4 for a typical case. If the "jump" passes the correct P then the subroutine automatically reduces the size of n to reduce the size of the next jump. This technique appreciably reduces the amount of computer time required. See section on results and conclusions.

A brief flow diagram is in Appendix E and a computer listing of this subroutine is given in Appendix F.

RESULTS AND CONCLUSIONS

In order to calculate the amount of computer time which can be saved by the various changes incorporated into the program, four runs were made for a short sphere-cone body in $M_\infty = 22$ flow. Initially the program was run to $X_{max} = 2$ nose radii using the original program. Secondly the improvements made in subroutine ISENC were added and the program rerun. This reduces the required run time from 246.1 seconds to 158.6 seconds as shown in Table 1. Then corrections in SERCH were included and rerun. An additional 92 seconds of run time (Table 1) were saved. Finally the program was run with all improvements including those in RGAS. The percentages given in Table 1 are based on the current run compared with the previous run. Comparing the final run time with the original program, a savings of 79% in computer time is realized. Considering a longer body ($X_{max} = 60$) a savings of 89% is realized. Results obtained with the improved method were identical to those obtained with the original program.

Therefore, it is of great importance that the original subroutines be modified if the program is to be used to obtain real equilibrium gas flow fields.

TABLE 1

Computer Times Required for the Program in Various Stages of Improvement. ($X_{max} = 2$, $M_\infty = 22$)

Type of Program	Time (sec)	Time Saving (sec)	%
Original Program	246.1	-	-
Improved ISENC Sub.	158.6	87.5	36%
Improved ISENC and SERCH Sub.	66.4	92.2	58%
Improved ISENC, SERCH and RGAS Sub.	51.2	15.2	23%

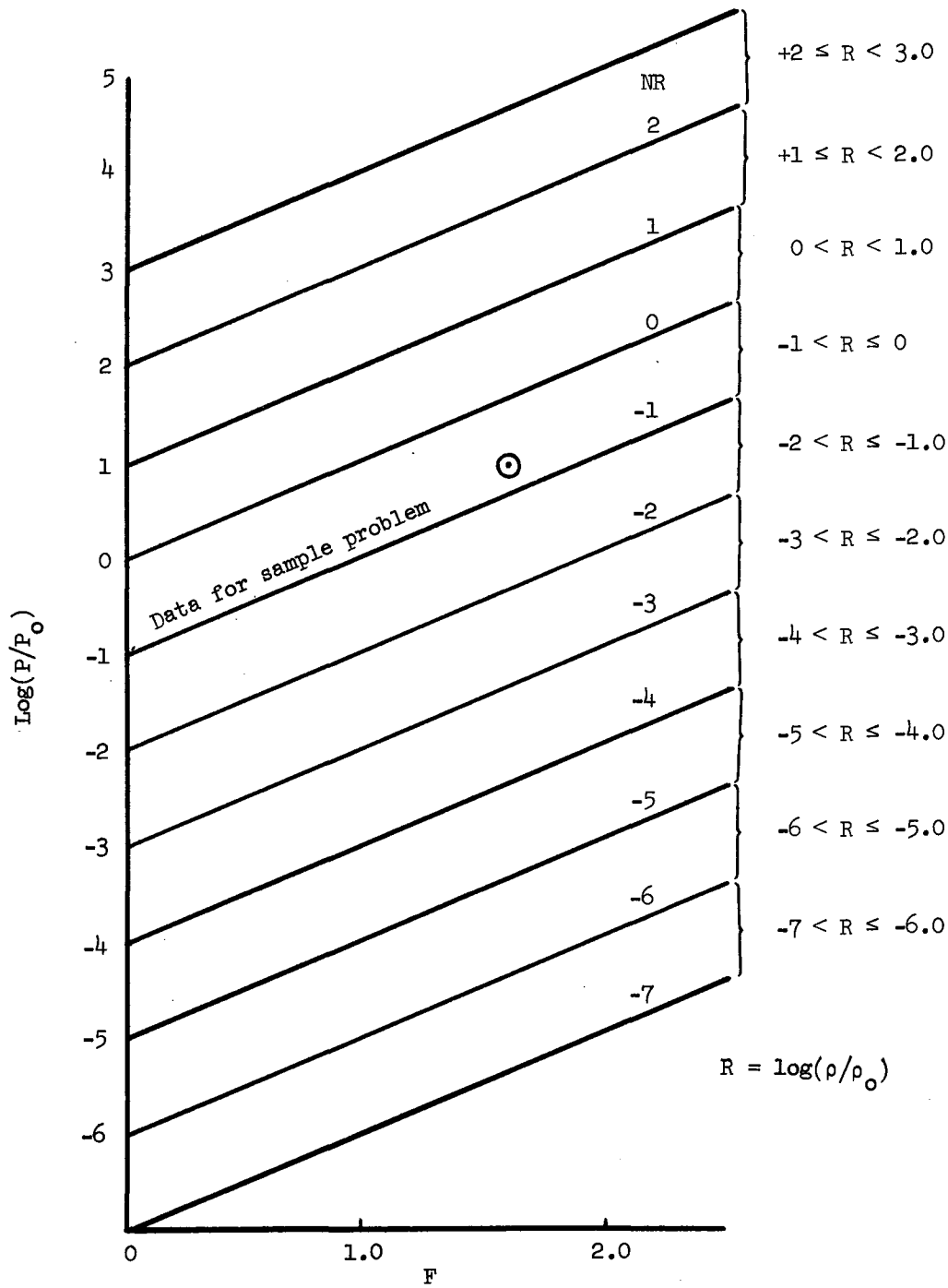

Figure 1. Function F Determined from Pressure and Density.

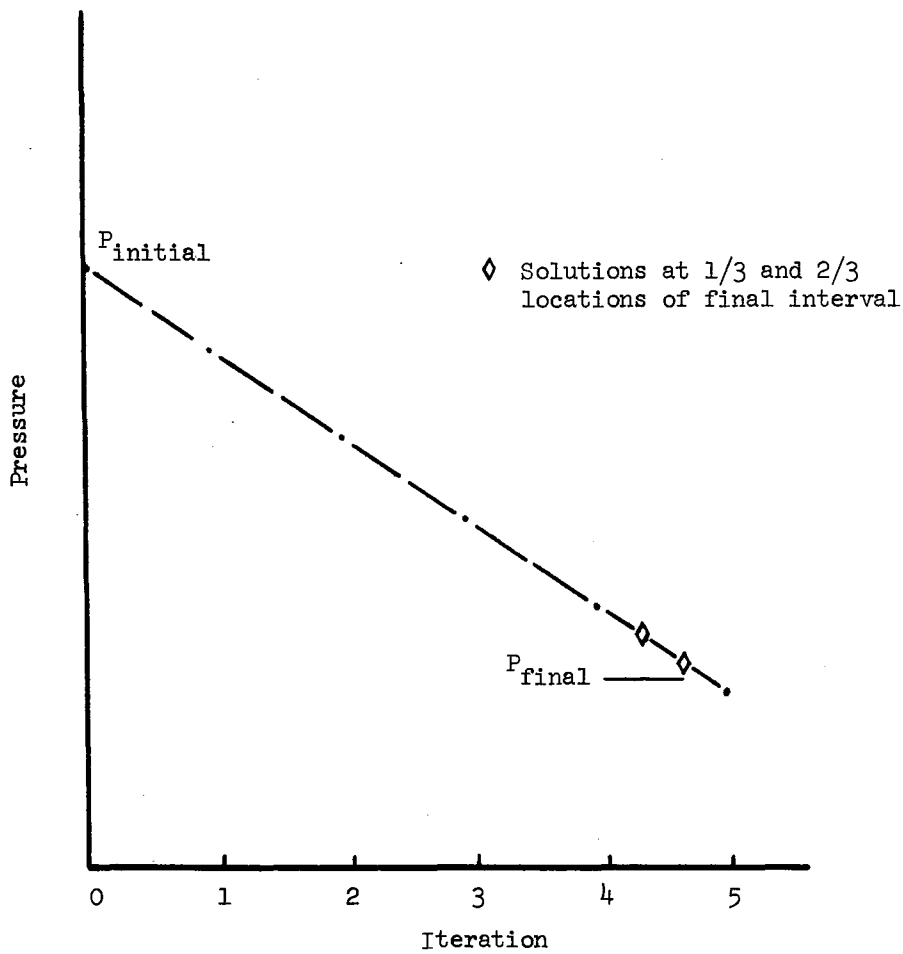

Figure 2. Iterative Sequence for $P_{initial}$ Larger than P_{final}.

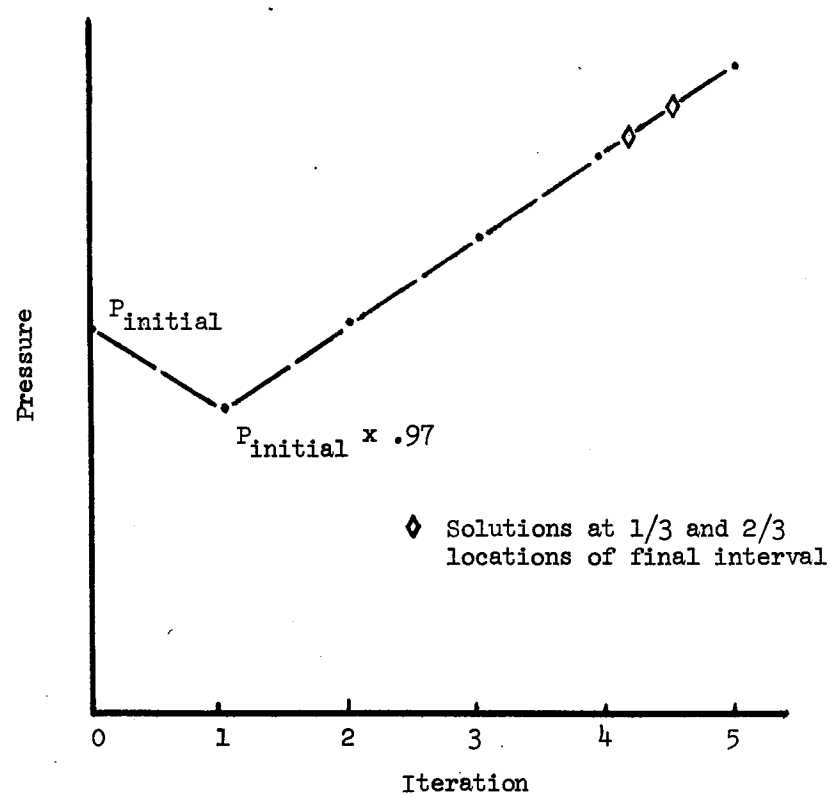

Figure 3. Iterative Sequence for $P_{initial}$ Smaller than P_{final}.

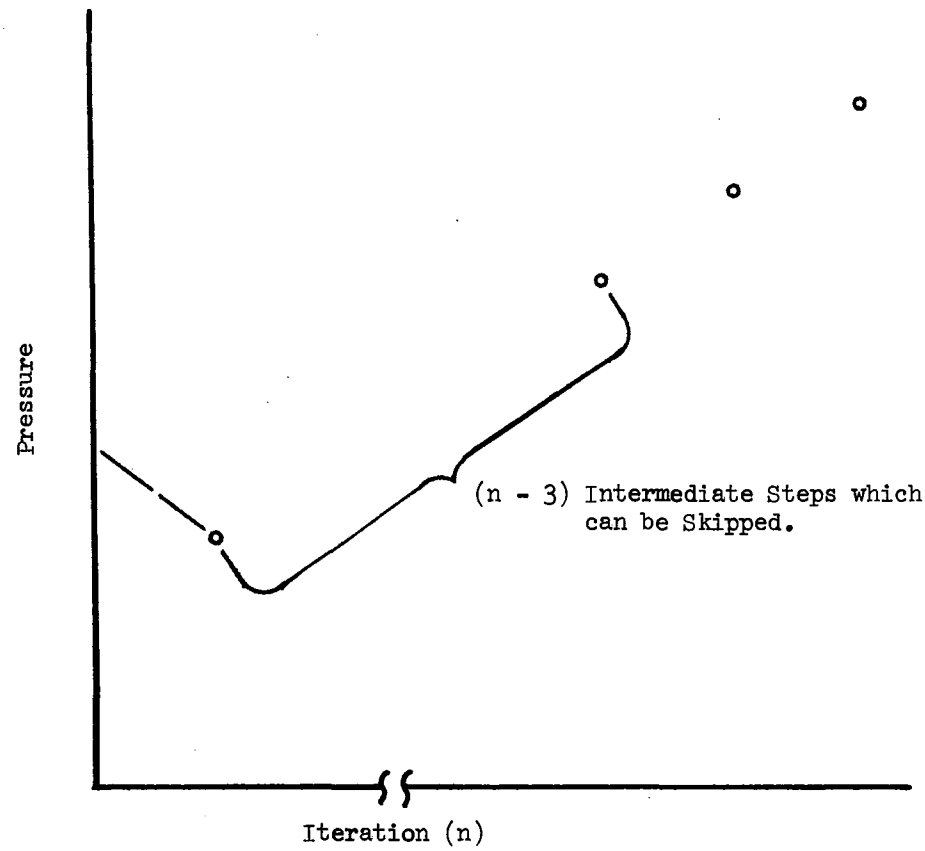

Figure 4. Sequence for $P_{initial}$ Smaller than P_{final} and (n - 3) Steps Skipped.

REFERENCES

1. Eaton, R. R. and Larson, D. E., "A Description of the Sandia version of the NASA-Ames Flow Field Code. Input-Output and Storage Locations," Sandia Laboratories, Albuquerque, New Mexico, SAND74-0096, November 1974.

APPENDIX A

SAMPLE CASE ILLUSTRATING OPERATION OF RGAS

The mechanics of subroutine RGAS are illustrated through the use of a sample case. It is assumed that the subroutine is entered with a pressure of 18599.449 psfa and density of 0.0005689099724 slugs/ft^3, and the property index NUMX is equal to 4. Base 10 logarithms of normalized pressure (51)* and density (73) are used in RGAS. The applicable normalizing parameters are listed in Appendix B under line numbers 35-50. Thus, P equals .943984427646 and R is -0.6409352834.

Array TH consists of a series of "boxes" containing the desired coefficients for all four output variables. The specific set of coefficients is located by comparing F(89) with the indexing parameters in the corresponding boxes of the TH5 array. Arrays NDL and NDU define the beginning and end position respectively of each box in TH and TH5. Table A1 lists the directory information contained in NDL and NDU for each of the four output variables. The NR + 8 position is determined by the value of R which spans the range of $-7 < R < 3$. Table A2 contains a listing of the beginning portion of TH and TH5.

For the sample case NR(79-86) equals -1. The calculated value of F, 1.595155586, is used to search TH5 from 120 to 129 for sonic velocity data. This search, which is done in SERCH, can be verified by comparing the value of F against those in Table A2 from TH5(120) to TH5(129). The value nearest to but less than F is 1.3687 which means NOUT is 125. Thus the polynomial coefficients are TH(1,125), TH(2,125), TH(3,125) and TH(4,125). The resulting polynomial is solved as a function of F to give Y1 equal to 6.749088. The Do Loop which enters the final answer in AN(N1) is from line 97 to 109. The normalized values of the state properties, which were described in the body of the report as lying between two boxes, are calculated linearly a DX(87) distance between Y1 and Y2 (108). Results for this case and the remaining three output variables are listed in Table A3. Further insight can be obtained from Figure A1 which is a plot

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*Numbers in the ( ) refer to specific Fortran logic statements in Appendix C.

of the two boxes involved for the sonic speed property. The solutions for F are shown at Y1 and Y2 with the solution of AN(1) (not shown) located at 6.66 between them. Final answers are obtained from the intermediate results by using the dimensionalizing constants given from statement numbers 114 to 117.

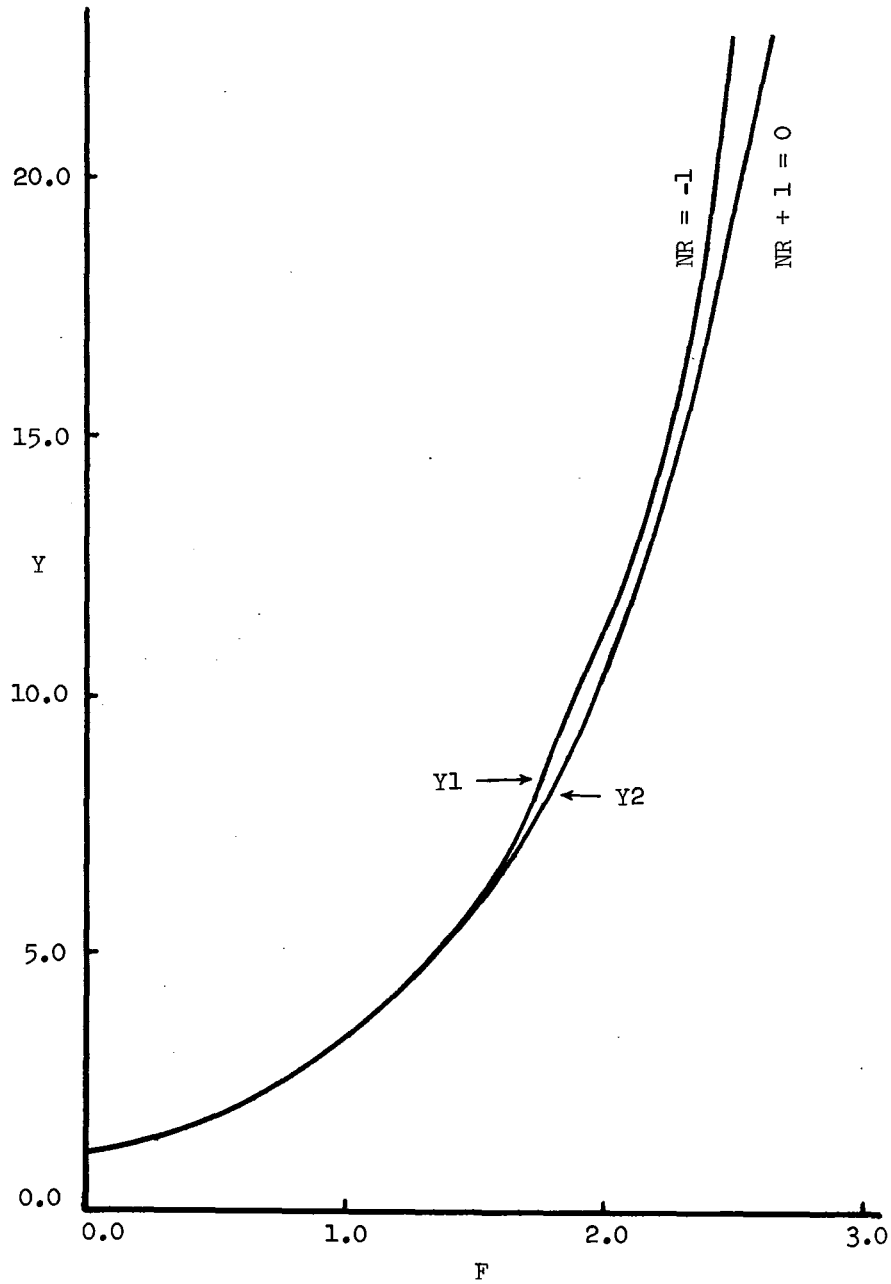


Figure A1. Calculated Y Curves for Sonic Speed (Air) Using TH Coefficients Obtained from Table 2A.

Table A1

Directory Information, in Arrays NDL and NDU, Used to Address Sets of Real Gas Data in Array TH

	N1 = 1 Sonic Velocity		N1 = 2 Enthalpy		N1 = 3 Temperature		N1 = 4 Entropy	
(NR + 8)	NDL	NDU	NDL	NDU	NDL	NDU	NDL	NDU
1	1	26	156	177	300	314	422	434
2	27	49	178	196	315	328	435	446
3	50	68	197	212	329	341	447	457
4	69	88	213	227	342	353	458	468
5	89	105	228	241	354	366	469	478
6	106	119	242	253	367	378	479	487
7	120	129	254	264	379	389	488	494
8	130	137	265	274	390	399	495	500
9	138	144	275	284	400	408	501	505
10	145	150	285	292	409	415	506	509
11	151	155	293	299	416	421	510	512

Table A2

Polynomial Coefficients, Stored in TH Array, for Spline Fits of the Real Gas Properties; Sonic Velocity, Enthalpy, Temperature and Entropy

Spline Fit Coefficients (TH Array)				Index Parameters (TH5)	
1.1358E+00	1.4134E+00	9.3266E-01	2.1549E-01	0.	1
-1.9072E+00	9.6979E+00	-2.0497E+00	-3.6998E+00	6.0833E-01	3
2.2244E+01	-6.9682E+01	7.9186E+01	-2.8116E+01	7.8575E-01	5
8.0561E+02	-2.5685E+03	2.7308E+03	-9.6395E+02	9.1249E-01	7
-6.7693E+01	2.2380E+02	-2.3202E+02	7.9910E+01	1.0392E+00	9
-4.2154E+02	9.7038E+02	-7.4061E+02	1.8977E+02	1.2927E+00	11
6.6843E+03	-1.4201E+04	1.0054E+04	-2.3696E+03	1.3941E+00	13
9.0455E+02	-1.6845E+03	1.0485E+03	-2.1629E+02	1.4955E+00	15
-3.1055E+03	5.0163E+03	-2.6994E+03	4.8564E+02	1.8503E+00	17
1.9712E+04	-2.9777E+04	1.4982E+04	-2.5090E+03	1.9771E+00	19
-4.8051E+04	6.9701E+04	-3.2723E+04	5.1941E+03	2.1038E+00	21
-2.9384E+02	4.2735E+02	-2.0544E+02	3.4261E+01	2.2052E+00	23
3.3482E+04	-4.1066E+04	1.6771E+04	-2.2789E+03	2.4333E+00	25
1.1356E+00	1.4092E+00	8.6545E-01	3.2943E-01	0.	27
6.9568E+00	-3.5601E+01	7.1932E+01	-4.2656E+01	6.8437E-01	29
-1.1152E+01	5.0841E+01	-6.5047E+01	2.9130E+01	8.1110E-01	31
1.0025E+03	-3.0653E+03	3.1258E+03	-1.0591E+03	9.6318E-01	33
1.2564E+02	-3.0337E+02	2.4861E+02	-6.6554E+01	1.0899E+00	35
-1.0620E+03	2.3368E+03	-1.7102E+03	4.1854E+02	1.3941E+00	37
-6.1052E+03	1.1971E+04	-7.8163E+03	1.7014E+03	1.4955E+00	39
-3.2477E+01	6.5584E+01	-4.0824E+01	9.7124E+00	1.6729E+00	41
-1.9036E+03	3.1475E+03	-1.7247E+03	3.1512E+02	1.9771E+00	43
-4.3186E+04	6.0334E+04	-2.8080E+04	4.3554E+03	2.1038E+00	45
-7.5463E+02	1.0224E+03	-4.6085E+02	7.0678E+01	2.2559E+00	47
1.3718E+03	-1.0168E+03	1.3480E+02	2.2691E+01	2.4840E+00	49
1.1096E+00	1.6035E+00	3.5060E-01	7.1110E-01	5.3228E-01	51
-6.6956E+00	3.8159E+01	-5.2880E+01	2.5133E+01	7.8575E-01	53
6.9473E+02	-2.0453E+03	2.0094E+03	-6.5518E+02	9.8853E-01	55
1.2199E+02	-2.8345E+02	2.2369E+02	-5.7520E+01	1.1406E+00	57
-5.4576E+02	1.1882E+03	-8.5797E+02	2.0764E+02	1.4448E+00	59
-3.6533E+03	6.9016E+03	-4.3391E+03	9.0986E+02	1.5462E+00	61
-1.9382E+02	3.2399E+02	-1.7843E+02	3.4644E+01	1.7996E+00	63
2.5449E+04	-3.4203E+04	1.7150E+04	-2.7077E+03	2.1038E+00	65
1.2484E+04	-1.6131E+04	6.9483E+03	-9.9612E+02	2.2305E+00	67

Spline Fit Coefficients (TH Array)				Index Parameters (TH5)	
1.5821E+00	-6.2785E-02	1.7530E+00	9.2478E-01	5.3228E-01	2
-4.3795E+01	1.9088E+02	-2.6315E+02	1.2166E+02	7.0971E-01	4
-8.0921E+02	2.7478E+03	-3.1033E+03	1.1701E+03	8.8714E-01	6
-8.1065E+02	2.3678E+03	-2.2944E+03	7.4120E+02	9.8853E-01	8
2.4001E+01	-5.1546E+01	4.0595E+01	-9.2608E+00	1.1153E+00	10
-3.2843E+03	7.2720E+03	-5.3644E+03	1.3206E+03	1.3687E+00	12
-6.2203E+03	1.2546E+04	-8.4254E+03	1.8861E+03	1.4448E+00	14
-2.3185E+01	5.0234E+01	-3.2526E+01	8.2605E+00	1.6222E+00	16
7.1096E+02	-7.5966E+02	2.1195E+02	-3.0861E+00	1.9264E+00	18
-3.4509E+04	4.9232E+04	-2.3393E+04	3.7041E+03	2.0531E+00	20
2.0116E+04	-2.7513E+04	1.2544E+04	-1.9049E+03	2.1291E+00	22
-2.3071E+04	2.9518E+04	-1.2590E+04	1.7918E+03	2.3573E+00	24
-9.2285E+02	1.1023E+03	-4.5316E+02	6.5821E+01	2.4840E+00	26
1.8593E+00	-2.5097E+00	7.8784E+00	-3.8100E+00	5.0694E-01	28
-3.7151E+01	1.6111E+02	-2.1838E+02	9.9291E+01	7.3506E-01	30
-3.9118E+02	1.2830E+03	-1.3965E+03	5.0862E+02	9.3783E-01	32
-7.7662E+02	2.1857E+03	-2.0402E+03	6.3499E+02	1.0139E+00	34
-4.7799E+01	1.1795E+02	-9.2529E+01	2.5515E+01	1.2420E+00	36
5.3184E+03	-1.0980E+04	7.5549E+03	-1.7300E+03	1.4448E+00	38
7.3953E+02	-1.3330E+03	8.0367E+02	-1.6024E+02	1.5462E+00	40
-2.5909E+03	4.0837E+03	-2.1444E+03	3.7678E+02	1.9010E+00	42
2.5708E+04	-3.7735E+04	1.8453E+04	-3.0043E+03	2.0278E+00	44
1.7491E+04	-2.3352E+04	1.0393E+04	-1.5403E+03	2.1798E+00	46
-2.9994E+04	3.7380E+04	-1.5530E+04	2.1527E+03	2.4080E+00	48
1.1356E+00	1.3984E+00	8.4610E-01	3.3178E-01	0.	50
-6.4230E+00	2.7481E+01	-2.7024E+01	8.9609E+00	6.8437E-01	52
-5.5643E+01	1.9335E+02	-2.1617E+02	8.2111E+01	8.8714E-01	54
-7.5756E+02	2.0475E+03	-1.8353E+03	5.4871E+02	1.0646E+00	56
-6.7208E+01	1.5771E+02	-1.1919E+02	3.1307E+01	1.2927E+00	58
4.3793E+03	-8.7473E+03	5.8230E+03	-1.2898E+03	1.4955E+00	60
2.7973E+02	-4.6819E+02	2.6331E+02	-4.8059E+01	1.6222E+00	62
-2.8969E+03	4.4194E+03	-2.2465E+03	3.8212E+02	2.0024E+00	64
-4.9900E+04	6.7782E+04	-3.8676E+04	4.6270E+03	2.1798E+00	66
-1.1097E+03	1.4467E+03	-6.2824E+02	9.2411E+01	2.3319E+00	68

Table A2 (Con't)

Spline Fit Coefficients (TH Array)				Index Parameters (TH5)	
1.1356E+00	1.3827E+00	8.3940E-01	2.9771E-01	0.	69
1.2093E+01	-4.6748E+01	7.1137E+01	-3.3833E+01	7.3506E-01	71
-5.1456E+00	2.7823E+01	-3.4787E+01	1.5653E+01	9.1249E-01	73
6.9352E+02	-1.9465E+03	1.8238E+03	-5.6717E+02	1.0646E+00	75
1.1273E+02	-2.5062E+02	1.8963E+02	-4.6566E+01	1.1913E+00	77
4.7416E+02	-8.8794E+02	5.5392E+02	-1.1317E+02	1.4955E+00	79
-1.9126E+03	3.4742E+03	-2.0981E+03	4.2306E+02	1.6222E+00	81
-5.0501E+02	7.8253E+02	-4.0264E+02	7.0367E+01	1.9264E+00	83
2.5456E+04	-3.4917E+04	1.5958E+04	-2.4283E+03	2.1798E+00	85
1.0499E+04	-1.3361E+04	5.5615E+03	-7.7020E+02	2.3066E+00	87
1.1356E+00	1.3622E+00	8.2095E-01	2.7503E-01	0.	89
-4.2729E+00	1.8509E+01	-1.6167E+01	5.2861E+00	7.6041E-01	91
1.9811E+02	-5.2795E+02	4.7225E+02	-1.3881E+02	1.0646E+00	93
3.2411E+01	-5.6555E+01	3.4478E+01	-5.5157E+00	1.2167E+00	95
-3.5144E+02	7.0062E+02	-4.6272E+02	1.0313E+02	1.5462E+00	97
-8.8781E+02	1.5413E+03	-8.8754E+02	1.7121E+02	1.6982E+00	99
-1.1741E+03	1.6913E+03	-8.1126E+02	1.3107E+02	2.0784E+00	101
3.6831E+03	-5.3381E+03	2.5481E+03	-3.9994E+02	2.3066E+00	103
9.6358E+02	-1.0785E+03	4.0134E+02	-4.8213E+01	2.4333E+00	105
1.8398E+00	-1.9854E+00	5.9047E+00	-2.2839E+00	5.5763E-01	107
-3.2257E-01	1.1715E+01	-1.5655E+01	7.7121E+00	1.0392E+00	109
-1.7550E+02	4.1330E+02	-3.1842E+02	8.2559E+01	1.2673E+00	111
-1.8328E+01	5.2306E+01	-4.1401E+01	1.1645E+01	1.5969E+00	113
-1.5298E+02	2.6403E+02	-1.4813E+02	2.8635E+01	1.7996E+00	115
-7.8028E+02	1.0810E+03	-4.9867E+02	7.8014E+01	2.2559E+00	117
8.1918E+03	-1.0113E+04	4.1641E+03	-5.7041E+02	2.4586E+00	119
1.5388E+00	-5.3265E-01	3.4681E+00	-1.0226E+00	5.5763E-01	121
3.0230E+01	-6.7511E+01	5.3570E+01	-1.2763E+01	1.1406E+00	123
1.8504E+01	-2.6110E+01	1.3703E+01	-1.2254E+00	1.3687E+00	125
-4.1489E+02	6.3528E+02	-3.2153E+02	5.5203E+01	1.8250E+00	127
-2.4394E+02	3.4091E+02	-1.5786E+02	2.5564E+01	2.3319E+00	129
1.4474E+00	-6.7854E-02	2.5629E+00	-5.6200E-01	5.8298E-01	131
6.2493E+01	-1.4225E+02	1.1145E+02	-2.7864E+01	1.3180E+00	133

Spline Fit Coefficients (TH Array)				Index Parameters (TH5)	
2.0111E+00	-3.0448E+00	8.2052E+00	-3.7188E+00	5.3228E-01	70
-1.8905E+01	7.8286E+01	-9.5816E+01	4.0039E+01	8.1110E-01	72
1.0272E+01	-4.2710E+00	-1.6472E+01	1.4017E+01	1.0139E+00	74
-6.8626E+02	1.7753E+03	-1.5225E+03	4.3575E+02	1.1153E+00	76
-5.7284E+01	1.3091E+02	-9.5761E+01	2.4593E+01	1.3434E+00	78
1.1796E+03	-2.3430E+03	1.5488E+03	-3.3883E+02	1.5715E+00	80
1.4129E+02	-2.1728E+02	1.1289E+02	-1.8236E+01	1.6982E+00	82
-1.8152E+03	2.7218E+03	-1.3581E+03	2.2710E+02	2.1038E+00	84
-4.7283E+04	6.2085E+04	-2.7162E+04	3.9608E+03	2.2559E+00	86
5.1241E+02	-5.8495E+02	2.2089E+02	-2.6063E+01	2.4080E+00	88
1.5681E+00	-7.5440E-01	4.1948E+00	-1.4604E+00	5.3228E-01	90
3.1203E+00	2.2250E+00	-7.6370E+00	5.7730E+00	8.8714E-01	92
-2.0334E+02	4.8287E+02	-3.7447E+02	9.7095E+01	1.1406E+00	94
-1.1412E+01	3.2213E+01	-2.4830E+01	7.5206E+00	1.3434E+00	96
1.6675E+03	-3.0823E+03	1.8995E+03	-3.8848E+02	1.6222E+00	98
4.4429E+01	-5.4331E+01	2.2225E+01	-1.5774E+00	1.7996E+00	100
1.1597E+04	-1.5312E+04	6.7334E+03	-9.8474E+02	2.2305E+00	102
-2.1165E+04	2.6683E+04	-1.1204E+04	1.5686E+03	2.3573E+00	104
1.1356E+00	1.3375E+00	7.8091E-01	2.7970E-01	0.	106
-1.8855E+01	6.7569E+01	-7.1669E+01	2.6406E+01	8.3645E-01	108
1.2696E+02	-3.3661E+02	3.0007E+02	-8.7157E+01	1.1913E+00	110
1.9108E+01	-2.9778E+01	1.7363E+01	-2.1573E+00	1.3687E+00	112
2.2121E+02	-4.3413E+02	2.8115E+02	-5.8534E+01	1.7236E+00	114
-6.8124E+01	1.1391E+02	-6.1128E+01	1.2054E+01	1.9517E+00	116
8.7647E+03	-1.1124E+04	4.7020E+03	-6.6052E+02	2.3826E+00	118
1.1356E+00	1.3080E+00	7.5597E-01	2.4676E-01	0.	120
-1.2616E+01	4.4373E+01	-4.3814E+01	1.5489E+01	8.8714E-01	122
-5.4371E+01	1.0950E+02	-6.7747E+01	1.4319E+01	1.2673E+00	124
3.2510E+01	-4.0236E+01	1.5770E+01	-4.0391E-01	1.6982E+00	126
1.7644E+01	-8.3872E+00	-2.5911E+00	2.5866E+00	1.9517E+00	128
1.1357E+00	1.2742E+00	7.1082E-01	2.3965E-01	0.	130
8.4285E-02	7.3994E+00	-7.8574E+00	3.7672E+00	1.0646E+00	132
-1.7960E+01	4.4220E+01	-3.1054E+01	8.1141E+00	1.4448E+00	134

Table A2 (Con't)

Spline Fit Coefficients (TH Array)				Index Parameters (TH5)		Spline Fit Coefficients (TH Array)				Index Parameters (TH5)	
-2.0874E+01	4.4816E+01	-2.8558E+01	7.0308E+00	1.6475E+00	135	-2.7403E+02	3.9393E+02	-1.8694E+02	3.0580E+01	1.9517E+00	136
-3.6211E+01	6.1931E+01	-3.2646E+01	6.7081E+00	2.3305E+00	137	1.1357E+00	1.2356E+00	6.6545E-01	2.2471E-01	0.	138
1.1671E+00	1.1576E+00	6.6758E-01	2.9269E-01	6.0833E-01	139	7.9766E-01	4.3401E+00	-4.0610E+00	2.2410E+00	1.1406E+00	140
1.1223E+01	-2.4150E+01	2.0719E+01	-4.7227E+00	1.3941E+00	141	-6.1021E+00	1.9135E+01	-1.3323E+01	3.8763E+00	1.5715E+00	142
1.8340E+02	-2.5972E+02	1.2341E+02	-1.8466E+01	2.0024E+00	143	-1.0019E+00	1.2382E+01	-9.1194E+00	2.8781E+00	2.2559E+00	144
1.1358E+00	1.1916E+00	6.2948E-01	1.8882E-01	0.	145	1.0524E+00	1.6076E+00	-6.2208E-02	5.7208E-01	6.0833E-01	146
1.0444E+00	2.5866E+00	-1.7240E+00	1.2822E+00	1.1660E+00	147	-1.8154E+01	3.5454E+01	-1.9927E+01	4.4983E+00	1.4955E+00	148
-7.3124E+00	2.0120E+01	-1.3025E+01	3.5382E+00	1.7489E+00	149	-1.1616E+02	1.4226E+02	-5.7552E+01	8.7554E+00	2.3066E+00	150
1.1357E+00	1.1445E+00	5.9747E-01	1.3866E-01	0.	151	1.0851E+00	1.4289E+00	6.8842E-02	4.6426E-01	5.8298E-01	152
1.4368E+00	1.2174E+00	-3.7138E-01	7.7574E-01	1.1406E+00	153	-2.0074E+01	3.7402E+01	-2.0384E+01	4.4008E+00	1.5969E+00	154
-8.3614E+00	2.1246E+01	-1.3030E+01	3.2986E+00	1.9771E+00	155	3.2035E+00	8.0853E+00	9.8407E+00	1.5976E+01	0.	156
2.1484E+00	1.8003E+01	-2.1161E+01	4.8192E+01	3.0416E-01	157	-7.4954E+01	3.9292E+02	-6.2677E+02	3.7303E+02	5.8298E-01	158
-6.9152E+02	3.2112E+03	-4.9209E+03	2.5539E+03	6.5902E-01	159	-1.3936E+03	6.1523E+03	-9.0250E+03	4.4617E+03	7.3506E-01	160
3.0934E+03	-1.0961E+04	1.2731E+04	-4.7579E+03	7.8575E-01	161	5.1151E+03	-1.8496E+04	2.2080E+04	-8.6188E+03	8.3645E-01	162
-9.7540E+03	2.9786E+04	-3.0168E+04	1.0224E+04	9.3783E-01	163	-1.5073E+04	4.5087E+04	-4.4828E+04	1.4901E+04	1.0139E+00	164
1.1425E+04	-2.7995E+04	2.2360E+04	-5.6880E+03	1.0899E+00	165	2.0165E+04	-4.8235E+04	3.7955E+04	-9.6853E+03	1.2420E+00	166
4.9501E+04	-1.1561E+05	8.9487E+04	-2.2815E+04	1.3434E+00	167	-1.2784E+05	2.6493E+05	-1.8264E+05	4.2036E+04	1.4194E+00	168
4.6061E+04	-7.9285E+04	4.4473E+04	-7.9113E+03	1.5208E+00	169	7.8894E+04	-1.3375E+05	7.4514E+04	-1.3420E+04	1.7236E+00	170
2.6760E+05	-4.4340E+05	2.4377E+05	-4.4242E+04	1.8757E+00	171	-4.3710E+05	6.4501E+05	-3.1640E+05	5.1833E+04	1.9771E+00	172
-1.8333E+06	2.6704E+06	-1.2957E+06	2.0967E+05	2.0784E+00	173	1.1172E+06	-1.4836E+06	6.5348E+05	-9.5170E+04	2.1545E+00	174
1.2164E+06	-1.5981E+06	6.9671E+05	-1.0047E+05	2.2812E+00	175	-6.9833E+05	7.5775E+05	-2.6899E+05	3.1406E+04	2.3826E+00	176
-1.7952E+06	2.1511E+06	-8.5808E+05	1.1430E+05	2.4586E+00	177	3.2035E+00	8.0599E+00	9.7527E+00	1.5594E+01	0.	178
2.2466E+00	1.7135E+01	-1.8892E+01	4.5678E+01	3.0416E-01	179	-5.1932E+01	2.7915E+02	-4.4109E+02	2.7236E+02	6.0833E-01	180
-1.5297E+03	6.5345E+03	-9.2674E+03	4.4237E+03	7.0971E-01	181	1.1324E+03	-3.6370E+03	3.6871E+03	-1.0760E+03	7.8575E-01	182
6.6038E+03	-2.2680E+04	2.5780E+04	-9.6198E+03	8.6179E-01	183	-1.3678E+03	2.7648E+03	-1.2925E+03	-1.8365E+01	9.3783E-01	184
-1.0401E+04	3.0634E+04	-2.9943E+04	9.7974E+03	9.8853E-01	185	1.1593E+03	-3.2860E+02	-2.3233E+03	1.5912E+03	1.0899E+00	186
1.0561E+04	-2.4994E+04	1.9238E+04	-4.6893E+03	1.1660E+00	187	6.7902E+04	-1.5127E+05	1.1194E+05	-2.7371E+04	1.3687E+00	188
-1.4744E+05	2.9670E+05	-1.9870E+05	4.4429E+04	1.4448E+00	189	3.8159E+04	-6.3039E+04	3.3721E+04	-5.6249E+03	1.5462E+00	190
2.8257E+05	-4.5245E+05	2.4053E+05	-4.2235E+04	1.8757E+00	191	-5.6359E+05	8.1082E+05	-3.8809E+05	6.2026E+04	2.0278E+00	192
-1.4925E+06	2.1354E+06	-1.0176E+06	1.6173E+05	2.1291E+00	193	1.0490E+06	-1.3590E+06	5.8381E+05	-8.2864E+04	2.2052E+00	194
1.6315E+06	-2.0863E+06	8.8618E+05	-1.2473E+05	2.3319E+00	195	-1.6732E+05	9.0103E+04	8.4966E+03	-6.7539E+03	2.4586E+00	196
3.2035E+00	7.9970E+00	9.6216E+00	1.5158E+01	0.	197	2.2934E+00	1.6641E+01	-1.7709E+01	4.3915E+01	3.0416E-01	198
-4.4969E+01	2.4148E+02	-3.7378E+02	2.3160E+02	6.0833E-01	199	-1.0157E+03	4.2257E+03	-5.8245E+03	2.7171E+03	7.3506E-01	200

Table A3

Data Extracted from Tables A1 and A2 to Obtain Intermediate Results for Sample Case

		NR + 8 = 7			NR + 9 = 8			Intermediate Results
	N1	NL = NDL(N1,7)	NU = NDU(N1,7)	Y1	NL = NDL(N1,8)	NU = NDU(N1,8)	Y2	AN(N1)
Normalized Sonic = AN(1) Velocity	1	120	129	6.749088	130	137	6.495157	6.657908
Normalized Enthalpy = AN(2)	2	254	264	293.914313	265	274	223.05058	268.4696
Temperature = AN(3)	3	379	389	7236.71625	390	399	7429.264	7305.85335
Entropy = AN(4)	4	488	494	44.6211646	495	500	38.90891	42.57009

APPENDIX B

FUNCTIONAL DESCRIPTION OF RGAS BY LINE NUMBERS

Line No.	
10-14	Local variables are set equal to subroutine input parameters. NUM(NUMX) is either 4 and NUM5 is -1 with density and pressure input or NUM = 5 and NUM5 = 0 for pressure and entropy (S) input.
15	NTEST is negative for real gas. If zero or positive, ideal equations are used from Line 233, to the end. Real gas calculations are from 16 to 232.
16-50	Real gas data read in once, and many parameters initialized.
19-21	Read in from real gas tape (Tape 9) NDL, equivalence NDU, TH, WTMIX and C(1)-C(7).
23-24	Find and store the midpoint location between each NDL and NDU set in MIDL. This revision in SERCH allows a maximum of only half the distance from NDU to NDL to be searched in SERCH.
25-27	TH(5,N) data is stored in TH5(N), against which F is searched in SERCH. This single dimensioned array permits a faster more direct solution than the original method.
28-34	This coding originally was at 220 and is used whenever $F \leq 0.0$. The constant coefficients for each of the 4 variables, which is the solution for Y at F = 0, need to be determined only once and are stored in SAVFO for use at 220.
35-50	Many parameters are initialized here. To aid the discussion of the sample case (page 18) the significant variables will be identified for air, which is file 2 of Table 1, page 15, of Ref. 1.

Line No.

CONC =	.99629144514	(air)	
PO =	2116.		Normalizing parameter for pressure
RO =	.002488736	(air)	Normalizing parameter for density
B =	-.037985802	(air)	
E =	-.02828552	(air)	
D =	-.0017838726	(air)	
FM =	2.508714	(air)	Maximum value of F

51 Base 10 logarithm of input pressure normalized by PO is the value of P.

52 Branch on (NUM-5): For NUM = 4, to 73-77; for NUM = 5, to 53-72; for NUM = 6 (impossible branch), terminate at 205.

53-72 NUM = 5 branch. P and S input provided.

53-55 RGAS will solve for correct R (normalized logarithm of density). Initial R is calculated at 55. Solving Do Loop 97-109 for entropy and iterating on incremented values of R, the proper solution is obtained when the calculated entropy (119-120) matches input entropy, REAL, (normalized entropy, S/RRR).

56-58 When RGAS is called from a subroutine which is iterating to the solution of some variable, R converges with fewer iterations if the solution is initiated using R from the previous call (stored in RLAST, 127) to RGAS instead of the calculated R(55). This is normally the case if the calculated value of R varies less than 10% from the calculated value on the previous call and R is set to equal RLAST. If more than 10% variation exists, the calculated value is used to begin the solution.

59-65 The minimum (RH) and maximum (RL) allowable range for R is established. RH is calculated at 60-61. The maximum value of RL(59) is calculated by solving the equation of F(59) for R with F = 0 (see Figure 1). RH, RL and R must be within the range of -7.0 to 3.0.

66-72 Integer flags are set including NUMM = 5, NUMM9P = NUMM - 9 + NUM = 1, NBOT = 4 and NUP = 4. The last two provide that the calculating Do 17 Loop, 97-109, only calculates entropy until final value of R is achieved.

Line No.

73-77 NUM = 4 branch. P and R input provided. The logarithm of the input density normalized by RO is the value of R. NUMM = 5 and NUM9P = NUMM - 9 + NUM = 0, which will solve for all 4 variables (NBOT = 1 to NUP = 4) at one pass.

78-86 NR is determined from R. If R is positive, NR is integer value of R. Otherwise, NR = R - 1.0. $-7 \leq NR \leq 2$.

87-89 DX is the difference between R and NR. This is used to linearily interpolate between Y1 and Y2 which is calculated for F from coefficients from NR and NR + 1 respectively (108).

NR = NR + 8, provides positive integers 1-10 which can be used to address arrays NDL and NDU.

F is the variable used to search the TH5 RGAS data and is a function of variables P and R and constants B, E and D. See Figure 1 for the relationship of P, R, NR and F.

90 For F zero or positive go to 92.

91 For negative F, test that the value is nearly zero and if the absolute value is less than 10^{-8}, set F = 0.

94 Test NUMM9P. If $\neq 0$, go to 97. This branch is taken only for NUM = 5 when iterating to the solution of R.

95-96 Branch here for NUMM9P = 0. Always branch here for NUM = 4 and for NUM = 5 after final value of R is obtained. These tests determine if F is within the proper limits. If $F \leq 0$, branching is to 207 for the calculation of the 4 output variables. If F is too large, that is greater than FM(45), branching is to 186 for error message and termination.

97-109 This is the heart of RGAS which solves for up to 4 output variables and stores the normalized results in array AN.

AN(1) Normalized sonic velocity

AN(2) Normalized enthalpy, H

Line No.

AN(3) Temperature ^{o}K

AN(4) Normalized entropy, S

Refer to the preceeding discussion for details (page 18). Subroutine SERCH searches RGAS data from TH5(NL) to TH5(NU) (also stored and used in Q) for the location exceeding or equal to F(89). The coefficients for the preceeding position (NOUT) are used to solve the third degree polynomial for Y1 at F. Y2 is found in the same manner using NDL(N1, NR+1) and NDU(N1,NR+1) for NL and NU. The answer is obtained by linearly interpolating between Y1 and Y2 and is placed in AN(N1) (108,87).

110 Branch on NUM-5. For NUM = 4 go to 113, leave RX unchanged, and output final answers.

111 Branch to here for NUM = 5. If still iterating on R(NUMM9P $\neq$ 0) go to 119 to test again on entropy.

112 Branch here for NUM = 5 and final R found and calculate density from R.

113-118 Calculate final values of sonic velocity, enthalpy, temperature (^{o}R) and entropy and exit from RGAS.

119-120 Calculate (percentage) difference between input entropy and calculated value and determine if within tolerance (10^{-4}), then branch to 122 or 129.

122-128 Branch here when difference is within tolerance and prepare for one final pass through (97-109) Do Loop to calculate AN(1)-AN(3). AN(4) is supplied with normalized input S, and RLAST is set equal to final R.

129-185 Branch here when convergence not obtained and calculate a new value of R.

131 Convergence must be obtained within 20 iterations or branch to 186, print error message, and exit from RGAS.

132-185 Value of R is adjusted by adding .3, -.3, or linearly interpolating between solutions of the last two iterations (151,155). R is always kept within the limits of RH to RL(59-65).

186-206 This point is entered from 96 to 131 for error message and exit from RGAS. However, if F is negative or zero, branching will go to 207 for calculation of 4 output variables and density. For positive F an error message with the values of some of the variables are printed.

Line No.	
200-206	A maximum of nine calls to RGAS can pass through this error message and exit RGAS without changing the values of any of the output variables. On the tenth time the program will be terminated by a CALL EXIT.
207-232	Solution for F zero or negative called from 95 and 186. The RGAS coefficients are solved once for R = 0 (28-34), stored in SAVFO, the output variables placed in BN(1)-BN(4) and ANR array positions calculated. Branching is next to the ideal gas solution (242-264) but for the ANR positions with L = 8.
233-241	Begin ideal gas solution called from 15 using parameter list input conditions, γ and density. Solutions of ANR positions are begun with L = 0.
242-264	Ideal gas solution is concluded here.
265-268	Normal exit from RGAS.

Appendix C. RGAS Fortran Listing


```
      SUBROUTINE RGAS(PX,RX,AX,HX,TX,SX,RRX,GX,NTEST,NUMX,NGAS)
CRGASR     WALKER     TEMP CONVERTED TO RANKINE
      DIMENSION TH(5,600),NDL(4,11),NDU(4,11),AN(4),C(7),ANR(17),BN(4)
      EQUIVALENCE(NDL(45),NDU)
      COMMON /CSERCH/  F, TH5(600), NL, NU, NOUT, NER
      DIMENSION MIDL(4,11),  SAVF0(4)
      DATA IF0   / 0 /
C
C
      P=PX
      S=SX
      R=RX
      NUM=NUMX
      NUM5 = NUM - 5
    3 IF(NTEST) 7,8,8
    7 IF (NFIRST-NGAS) 10,9,10
   10 NFIRST=NGAS
      CALL LOCATE(NGAS,9)
      READ (9) (NDL(N),N=1,89)
      NMM =NDL(89)
      READ (9) (TH(N),N=1,NMM),WTMIX,(C(N),N=1,7)
      REWIND 9
      DO 115 N=1,44
  115 MIDL(N) =     (NDL(N)+NDU(N))/2
      NDUMX = NDU(44)
      DO 120 N=1,NDUMX
  120 TH5(N) = TH(5,N)
      F=0.
      DO 21 N1=1,4
      NL=NDL(N1,1)
      NU=NDU(N1,1)
      NER = MIDL(N1,1)
      CALL SERCH
   21 SAVF0(N1) = TH(1,NOUT)
      CONC=WTMIX/28.966
      P0=2116.
      R0=.002498*CONC
      RRR=1716./CONC
      RRX=RRR
      RT0=RRR*493.635
      SQP0R0 = SQRT(R0/P0)
      B=TH(NMM-2)
      E=TH(NMM-1)
      D=TH(NMM)
      FM=2.1632+.3468*CONC
      AA=D*FM
      BB=E*FM+1.
      CCC=B+FM
      RLAST = 0.0
      RSTART = 100.0
    9 P =ALOG(P/P0)/2.3025851
      IF(NUM5)40,31,70
   31 REAL=S/RRR
      GG=(REAL-C(1)-C(2)*P)/(C(3)+P*(C(4)+P*C(5)))
      R=C(6)*GG+C(7)*P
```

```
SUBROUTINE  RGAS                                    CDC 6600 FTN V3.0-V34A OPT=1  03/10/75  11.37.59.      PAGE      2
                PER = ABS((RSTART - R) / R)                                          COUNT     145
                RSTART = R                                                           COUNT     146
                IF (PER.LT. 0.1) R = RLAST                                           COUNT     147
                RL=P-R                                                               COUNT     148
                CC=CCC-P                                                             COUNT     149
                RH=-CC*(1.+AA*CC/(BB*BB))/BB+.005                                    COUNT     150
                IF(RH .LT. -7.) RH = -7.0                                            COUNT     151
                IF (R .LT. RH) R = RH                                                COUNT     152
                IF(RL.GT.3.0) RL = 3.0                                               COUNT     153
                IF(RL .LT.R) R = RL                                                  COUNT     154
                NUMB=0                                                               COUNT     155
                NIMX=0                                                               COUNT     156
                NUMM=5                                                               COUNT     157
                NUMM9P = NUMM - 9 + NUM                                              COUNT     158
                NBOT = 4                                                             COUNT     159
                NUP = 4                                                              COUNT     160
                GO TO 42                                                             COUNT     161
             40 R = ALOG(R/R0)/2.3025851                                             COUNT     162
                NUMM=5                                                               COUNT     163
                NUMM9P = NUMM - 9 + NUM                                              COUNT     164
                NBOT=1                                                               COUNT     165
                NUP=NUM                                                              COUNT     166
             42 CONTINUE                                                             COUNT     167
                IF(R)11,12,13                                                        COUNT     168
             11 NR = R - 1.0                                                         COUNT     169
                IF (NR .LT.-7) NR= -7                                                COUNT     170
                GO TO 15                                                             COUNT     171
             12 NR = -1.0                                                            COUNT     172
                GO TO 15                                                             COUNT     173
             13 NR = R                                                               COUNT     174
                IF(NR.GT.2) NR = 2                                                   COUNT     175
             15 DX=R-FLOAT(NR)                                                       COUNT     176
                NR=NR+8                                                              COUNT     177
                F=(P-R-B)/(1.+R*(E+D*R))                                             COUNT     178
                IF(F)158,160,160                                                     COUNT     179
            158 IF (F .GT. -1.0E-08) F = 0.0                                         COUNT     180
            160 CONTINUE                                                             COUNT     181
          C                 IF(NUMM-9+NUM) 22,162,22    -------- IF(NUMM9P)         COUNT     182
                IF (NUMM9P)22,162,22                                                 COUNT     183
            162 IF(F-.000001) 27,161,161                                             COUNT     184
            161 IF(FM .LT. F) GO TO 44                                               COUNT     185
             22 DO 17 N1=NBOT,NUP                                                    COUNT     186
             36 NL=NDL(N1,NR)                                                        COUNT     187
                NU=NDU(N1,NR)                                                        COUNT     188
                NER = MIDL(N1,NR)                                                    COUNT     189
                CALL SERCH                                                           COUNT     190
                Y1 = TH(1,NOUT) +F*(TH(2,NOUT)+F*(TH(3,NOUT)+F*TH(4,NOUT)))          COUNT     191
                NL=NDL(N1,NR+1)                                                      COUNT     192
                NU=NDU(N1,NR+1)                                                      COUNT     193
                NER = MIDL(N1,NR+1)                                                  COUNT     194
                CALL SERCH                                                           COUNT     195
                Y2 = TH(1,NOUT) +F*(TH(2,NOUT)+F*(TH(3,NOUT)+F*TH(4,NOUT)))          COUNT     196
                AN(N1)=Y1+DX*(Y2-Y1)                                                 COUNT     197
             17 CONTINUE                                                             COUNT     198
                IF(NUM5 ) 51,52,52                                                   COUNT     199
```

```
SUBROUTINE  RGAS                                    CDC 6600 FTN V3.0-V34A OPT=1  03/10/75  11.37.59.      PAGE      3
                 52 IF(NUMM9P)39,108,39                                                    COUNT     200
                108 RX=R0*10.**R                                                           COUNT     201
                 51 GO TO (121,122,123,124,124),NUM                                        COUNT     202
                124 SX=AN(4)*RRR                                                           COUNT     203
                123  TX= AN(3)*1.8                                                         COUNT     204
                122 HX=AN(2)*RTO                                                           COUNT     205
                121 AX=AN(1)/SQPORO                                                        COUNT     206
                    GO TO 109                                                              COUNT     207
                 39   DIFF=ABS((REAL-AN(NUP))/REAL)                                       COUNT     208
                      IF(DIFF-.0001)  37,37,38                                             COUNT     209
              C                   NUMM9P = NUMM - 9 + NUM =  0                             COUNT     210
                 37 NUMM9P = 0                                                             COUNT     211
                    NUMM = 9 - NUM                                                         COUNT     212
                    NBOT=1                                                                 COUNT     213
                    NUP=3                                                                  COUNT     214
                    AN(4) = REAL                                                           COUNT     215
                    RLAST = R                                                              COUNT     216
                    GO TO 42                                                               COUNT     217
                 38 NUMB=NUMB+1                                                            COUNT     218
                    NIMX=NIMX+1                                                            COUNT     219
                    IF (NIMX .GT. 20) GO TO 44                                             COUNT     220
                 43 IF(NUMB-2)82,83,84                                                     COUNT     221
                 82 IF(REAL-AN(NUP)) 85,37,86                                              COUNT     222
                 85 R1=R                                                                   COUNT     223
                    S1=AN(NUP)                                                             COUNT     224
                    R=R+.3                                                                 COUNT     225
                    IF (RL.LT.R) R = RL                                                    COUNT     226
                    R2=R                                                                   COUNT     227
                    L = 0                                                                  COUNT     228
                    GO TO 42                                                               COUNT     229
                 86 R2=R                                                                   COUNT     230
                    S2=AN(NUP)                                                             COUNT     231
                    R=R-.3                                                                 COUNT     232
                    IF (R.LT.RH) R=RH                                                      COUNT     233
                    R1 = R                                                                 COUNT     234
                    L=1                                                                    COUNT     235
                    GO TO 42                                                               COUNT     236
                 83 IF(L) 91,90,91                                                         COUNT     237
                 90 S2=AN(NUP)                                                             COUNT     238
                    R=R2                                                                   COUNT     239
                    IF(S1.NE.S2) R=R2-(S2-REAL)/(S2-S1)*(R2-R1)                            COUNT     240
                    IF (RL.LT.R) R=RL                                                      COUNT     241
                    GO TO 93                                                               COUNT     242
                 91 S1=AN(NUP)                                                             COUNT     243
                    R=(REAL-S1      )/(S2-S1)*(R2-R1)+R1                                   COUNT     244
                    IF (R.LT.RH) R=RH                                                      COUNT     245
                 93 IF(R2-R) 104,37 ,105                                                   COUNT     246
                104 NUMB=1                                                                 COUNT     247
                    R1=R2                                                                  COUNT     248
                    S1=S2                                                                  COUNT     249
                    L=0                                                                    COUNT     250
                    IF(R2+.3-RL) 210,211,211                                               COUNT     251
                211 R2=RL                                                                  COUNT     252
                    R=R2                                                                   COUNT     253
                    GO TO 42                                                               COUNT     254
```

Appendix C (Continued)


```
  210 R2=R2+.3                                                    COUNT   255
      R=R2                                                        COUNT   256
      GO TO 42                                                    COUNT   257
  105 IF(R-R1) 106,37,42                                          COUNT   258
  106 NUMB=1                                                      COUNT   259
      R2=R1                                                       COUNT   260
      S2=S1                                                       COUNT   261
      L=1                                                         COUNT   262
      IF(RH-R1+.3) 212,213,213                                    COUNT   263
  213 R1=RH                                                       COUNT   264
      R=R1                                                        COUNT   265
      GO TO 42                                                    COUNT   266
  212 R1=R1-.3                                                    COUNT   267
      R=R1                                                        COUNT   268
      GO TO 42                                                    COUNT   269
   84 IF(REAL-AN(NUP)) 87,87,88                                   COUNT   270
   87 R1=R                                                        COUNT   271
      GO TO 91                                                    COUNT   272
   88 R2=R                                                        COUNT   273
      GO TO 90                                                    COUNT   274
   44 IF(F-.000001) 27,444,444                                    COUNT   275
  444 NTIMES=NTIMES+1                                             COUNT   276
      WRITE (6,190)                                               COUNT   277
  190 FORMAT(1H0,10X,36HOUTSIDE TABLES IN RGAS ENTERING WITH)     COUNT   278
      WRITE (6,191) PX                                            COUNT   279
  191 FORMAT(11X,2HP=,E13.6)                                      COUNT   280
      IF(NUMS ) 192,193,193                                       COUNT   281
  192 CONTINUE                                                    COUNT   282
      WRITE (6,194) RX                                            COUNT   283
  194 FORMAT(11X,2HR=E13.6)                                       COUNT   284
      GO TO 196                                                   COUNT   285
  193 CONTINUE                                                    COUNT   286
      WRITE (6,195) SX                                            COUNT   287
  195 FORMAT(11X,2HS=,E13.6)                                      COUNT   288
  196 IF(NTIMES-10) 109,197,197                                   COUNT   289
  197 CONTINUE                                                    COUNT   290
      WRITE (6,198)                                               COUNT   291
  198 FORMAT(20X,28HEXIT CALLED ON TENTH FAILURE)                 COUNT   292
      GO TO 25                                                    COUNT   293
   70 Z = Z*SQRT(-1.0)                                            COUNT   294
   25 CALL EXIT                                                   COUNT   295
   27 L=8                                                         COUNT   296
      P=PX                                                        COUNT   297
      R=RX                                                        COUNT   298
      IF (GTEST.EQ.GX) GO TO 440                                  COUNT   299
   24 GTEST= GX                                                   COUNT   300
      L1=9                                                        COUNT   301
      Z2=R0/10.**7                                                COUNT   302
      PR=-7.+B                                                    COUNT   303
      PR=P0*10.**PR                                               COUNT   304
      Z1=PR                                                       COUNT   305
      IF0 = IF0 + 1                                               COUNT   306
      F = 0.0                                                     COUNT   307
      DO 23 N1=1,4                                                COUNT   308
   23 AN(N1) = SAVF0(N1)                                          COUNT   309
```

Appendix C (Continued)

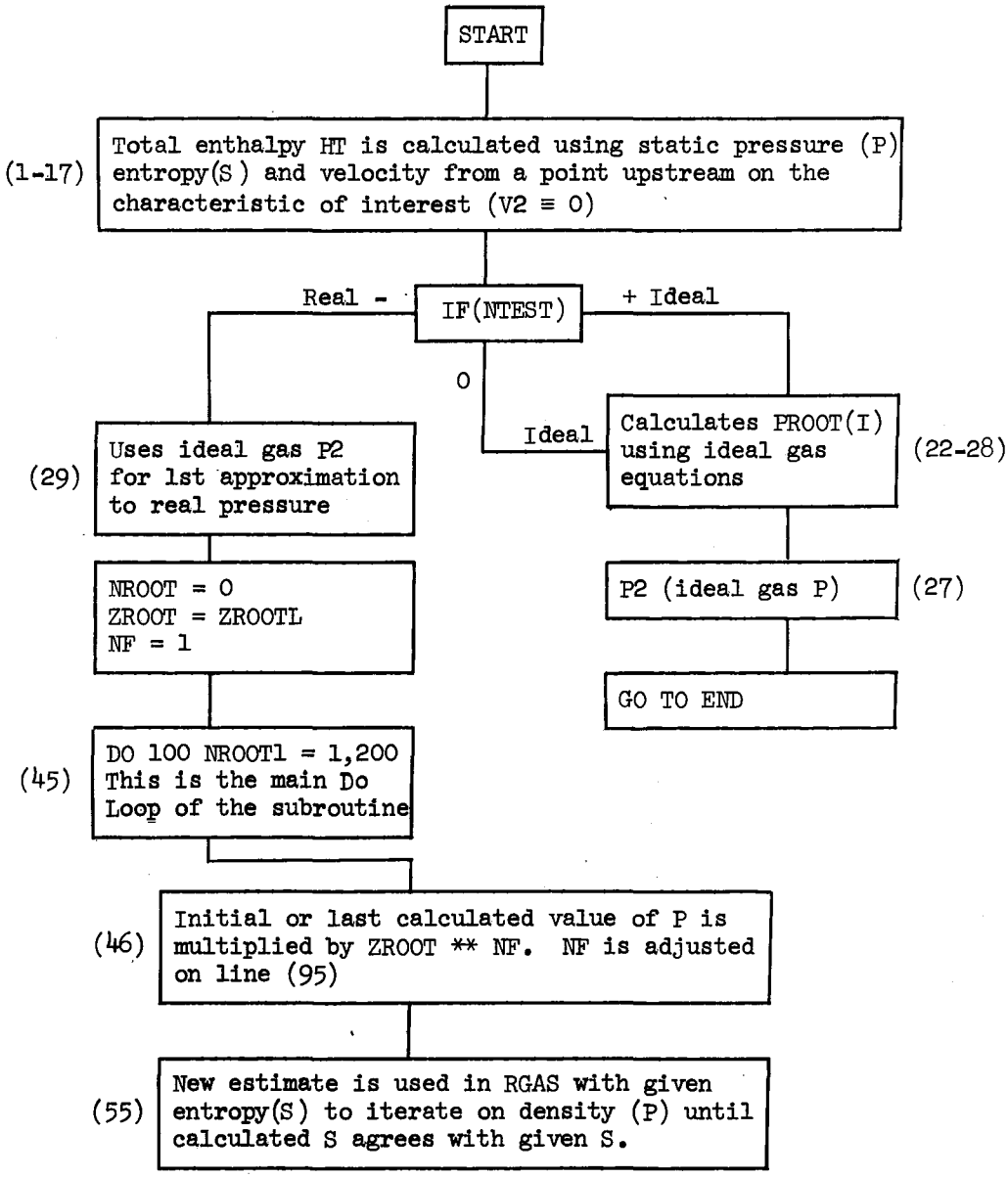

```
      BN(1)=BN(1)/SQPORO                                                COUNT   310
      BN(2)=BN(2)*RTO                                                   COUNT   311
      BN(3)=BN(3)*1.8                                                   COUNT   312
      BN(4)=BN(4)*RRR                                                   COUNT   313
      ANR(9)=PR/(Z2 *BN(3))                                             COUNT   314
      RRX=ANR(9)                                                        COUNT   315
      ANR(12)=BN(2)/BN (3)                                              COUNT   316
      ANR(10)=1.+ANR(9)/(ANR(12)-ANR(9))                                COUNT   317
      ANR(11)=ANR(12)/ANR(10)                                           COUNT   318
      ANR(17)=BN(1)*BN(1)*Z2/Z1                                         COUNT   319
      ANR(16)=BN(4)-ANR(11)*ALOG(Z1/Z2**ANR(10))                        COUNT   320
      GO TO 26                                                          COUNT   321
    8 L=0                                                               COUNT   322
      IF (GTEST.EQ.GX) GO TO 440                                        COUNT   323
   64 GTEST= GX                                                         COUNT   324
      L1=2                                                              COUNT   325
      ANR(1)=RRX                                                        COUNT   326
      ANR(2)=GX                                                         COUNT   327
      ANR(3)=ANR(1)/(ANR(2)-1.)                                         COUNT   328
      ANR(4)=ANR(1)+ANR(3)                                              COUNT   329
      ANR(8)=49008.609-ANR(3)*ALOG(171.6/.0001**ANR(2))                 COUNT   330
   26 ANR(L+5)=1./ANR(L+2)                                              COUNT   331
      ANR(L+6)=ANR(L+4)/ANR(L+1)                                        COUNT   332
      ANR(L+7)=ANR(L+6)/ANR(L+2)                                        COUNT   333
      IF(NUM5)440,69,70                                                 COUNT   334
  440 QUOD=P/R**ANR(L+2)                                                COUNT   335
      QUOT=P/R                                                          COUNT   336
      GO TO(65,66,67,68,69),NUM                                         COUNT   337
   69 EX=S-ANR(L+8)                                                     COUNT   338
      EX=EXP(EX/ANR(L+3))                                               COUNT   339
      R=(P/EX)**ANR(L+5)                                                COUNT   340
      QUOD=P/R**ANR(L+2)                                                COUNT   341
      QUOT=P/R                                                          COUNT   342
      GO TO 67                                                          COUNT   343
   68 S=ANR(L+8)+ANR(L+3)*ALOG(QUOD)                                    COUNT   344
   67 T=QUOT/ANR(L+1)                                                   COUNT   345
   66 H=QUOT*ANR(L+6)                                                   COUNT   346
   65 LL=L+L1                                                           COUNT   347
      A=SQRT(ANR(LL)*QUOT)                                              COUNT   348
   30 AX=A                                                              COUNT   349
      HX=H                                                              COUNT   350
      TX= T                                                             COUNT   351
      SX=S                                                              COUNT   352
      RX=R                                                              COUNT   353
  109 CONTINUE                                                          COUNT   354
      GTEST=-1.0E+30                                                    COUNT   355
      RETURN                                                            COUNT   356
      END                                                               COUNT   357
```

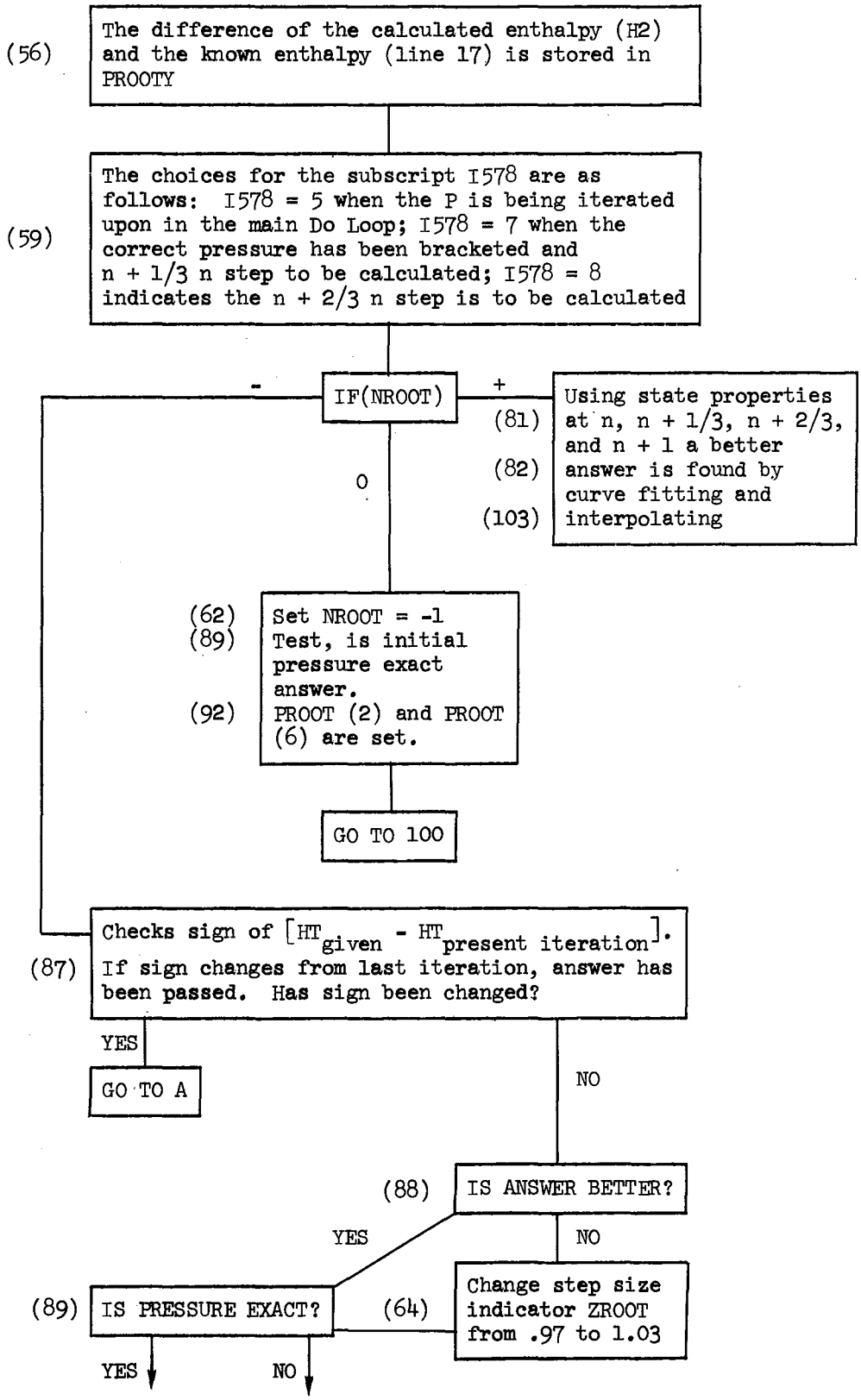
Appendix D. SERCH Fortran Listing

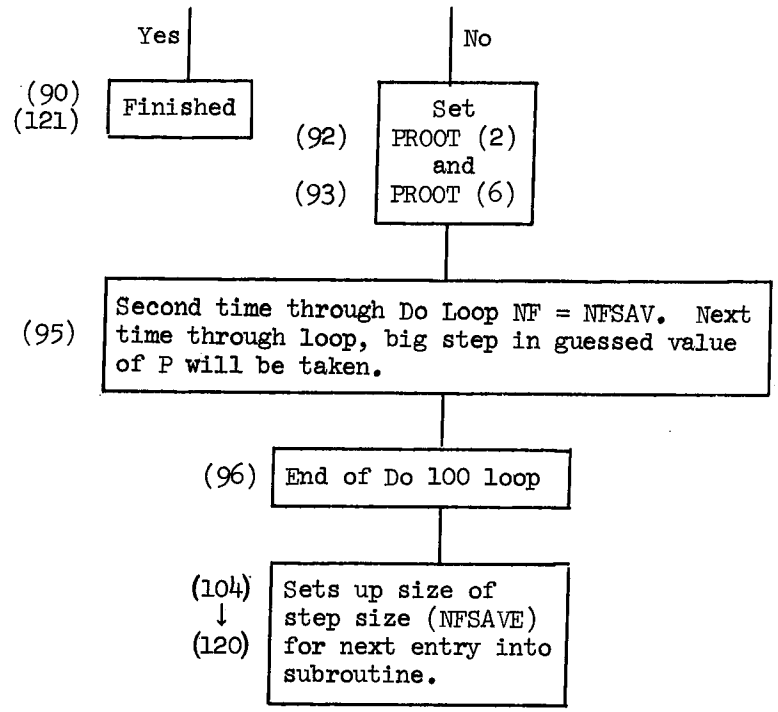
```
SUBROUTINE  SERCH                                   CDC 6600 FTN V3.0-V34A OPT=1  03/10/75  11.37.59.      PAGE      1

            SUBROUTINE SERCH                                                          COUNT     358
            COMMON /CSERCH/  X,   Q(600), NL, NU, NOUT, NER                           COUNT     359
            NOUT = 70000                                                              COUNT     360
            IF (X.GE. Q(NER)) NL=NER                                                  COUNT     361
            DO 10 I=NL,NU                                                             COUNT     362
            IF(X.LT. Q(I)) RETURN                                                     COUNT     363
            NOUT = I                                                                  SERCH      11
         10 CONTINUE                                                                  SERCH      12
            RETURN                                                                    COUNT     364
            END                                                                       COUNT     365
```

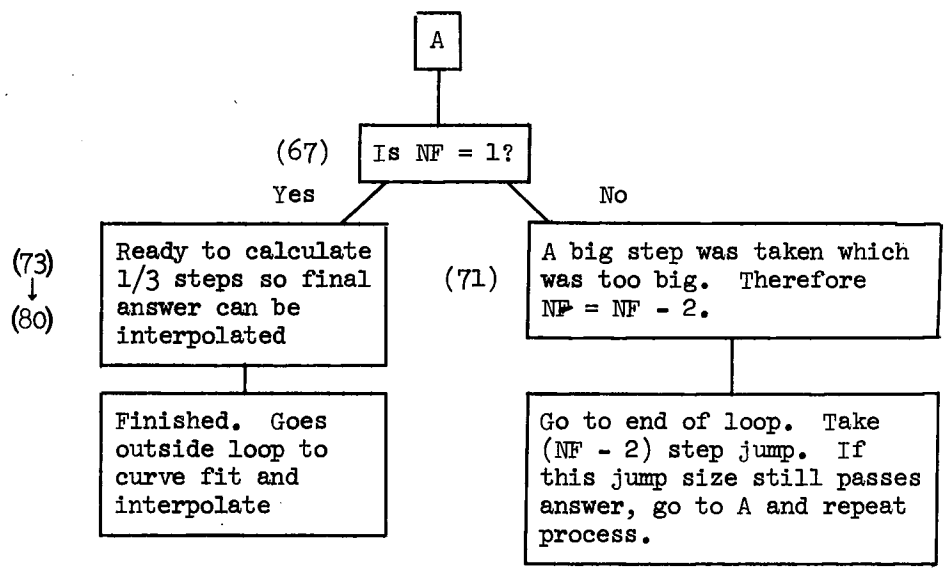
Appendix E

Subroutine ISENC Flow Diagram




(56)
The difference of the calculated enthalpy (H2) and the known enthalpy (line 17) is stored in PROOTY
(59)
The choices for the subscript I578 are as follows: I578 = 5 when the P is being iterated upon in the main Do Loop; I578 = 7 when the correct pressure has been bracketed and n + 1/3 n step to be calculated; I578 = 8 indicates the n + 2/3 n step is to be calculated
IF(NROOT)
-
+
0
(81)
(82)
(103)
Using state properties at n, n + 1/3, n + 2/3, and n + 1 a better answer is found by curve fitting and interpolating
(62)
(89)
(92)
Set NROOT = -1
Test, is initial pressure exact answer.
PROOT (2) and PROOT (6) are set.
GO TO 100
(87)
Checks sign of [HT given - HT present iteration].
If sign changes from last iteration, answer has been passed. Has sign been changed?
YES
GO TO A
NO
(88)
IS ANSWER BETTER?
YES
NO
(89)
IS PRESSURE EXACT?
(64)
Change step size indicator ZROOT from .97 to 1.03
YES
NO


Yes
No
(90)
(121)
Finished
(92)
(93)
Set PROOT (2) and PROOT (6)
(95)
Second time through Do Loop NF = NFSAV. Next time through loop, big step in guessed value of P will be taken.
(96)
End of Do 100 loop
(104)
↓
(120)
Sets up size of step size (NFSAVE) for next entry into subroutine.


A
(67)
Is NF = 1?
Yes
No
(73)
↓
(80)
Ready to calculate 1/3 steps so final answer can be interpolated
(71)
A big step was taken which was too big. Therefore NF = NF - 2.
Finished. Goes outside loop to curve fit and interpolate
Go to end of loop. Take (NF - 2) step jump. If this jump size still passes answer, go to A and repeat process.

Appendix F. ISENC Fortran Listing


```
      SUBROUTINE ISENC(P1,S1X,V1,V2,P2,RX,GX,NTESTX,NGASX,ER)          ISENC     2
CISENC     LOMAX                                                       ISENC     3
      DIMENSION PROOT(10)                                              ISENC     4
      DATA  NFSAV  / 1 /                                               COUNT     1
      DATA  LIMP1,  LIM,  LIM1  /  6, 5, 4  /                          COUNT     2
      DATA  ZROOTL /  .97  /                                           COUNT     3
      DATA  ZROOTH / 1.03 /                                            COUNT     4
C                                                                      ISENC     5
      ER=0.0                                                           ISENC     6
      R=RX                                                             ISENC     8
      G=GX                                                             ISENC     9
      NTEST=NTESTX                                                     ISENC    10
      NGAS=NGASX                                                       ISENC    11
      S1=S1X                                                           ISENC    12
      CALL RGAS(P1,R1,A1,H1,T1,S1,R,G,NTEST,S,NGAS)                    ISENC    13
      HT=H1+.5*V1**2                                                   ISENC    14
      HTMV2=HT-.5*V2**2                                                ISENC    15
      IF(HTMV2) 3,3,4                                                  ISENC    16
    3 ER=-1.0                                                          ISENC    17
      GO TO 5                                                          ISENC    18
    4 IF(NTEST) 6,7,7                                                  ISENC    19
    7 PROOT(1)=G/(G-1.)                                                ISENC    20
      PROOT(2)=(V1/A1)**2                                              ISENC    21
      PROOT(3)=(V2/A1)**2                                              ISENC    22
      PROOT(4)=PROOT(2)-PROOT(3)                                       ISENC    23
      PROOT(5)=(G-1.0)/2.0                                             ISENC    24
      P2=P1*(1.0+(PROOT(5)*PROOT(4)))**PROOT(1)                        ISENC    25
      GO TO 5                                                          ISENC    26
    6 PROOTX = P2                                                      COUNT     5
      IF(PROOTX) 1,1,2                                                 ISENC    30
    1 PROOTX=P1                                                        ISENC    31
    2       CONTINUE                                                   ISENC    32
C                                                                      ISENC    33
C                 PROOTX GUESSED VALUE OF ROOT                         ISENC    34
C                 ZROOTH AND ZROOTL PERCENT INCREMENTS                 ISENC    35
C                                                                      ISENC    36
      NROOT=0                                                          COUNT     6
      ZROOT =ZROOTL                                                    COUNT     7
      PROOT(9)=0.0                                                     COUNT     8
      MROOT = -1                                                       COUNT     9
      NFCHK = NFSAV                                                    COUNT    10
      NF = 1                                                           COUNT    11
      I578 = 5                                                         COUNT    12
      PROOT(1)=PROOTX/ZROOT                                            COUNT    13
      DO 100 NROOT1=1,200                                              COUNT    14
      PROOT(1) = PROOT(1)*ZROOT**NF                                    COUNT    15
      PROOTZ=PROOT(1)                                                  COUNT    16
  114 CONTINUE                                                         COUNT    17
C                                                                      COUNT    18
C                 INSERT EQUATION FOR ROOT                             COUNT    19
C                 PROOTZ = FUNCTION                                    COUNT    20
C                 PROOTY IS ZERO FOR TRUE ROOT                         COUNT    21
      JISENC = JISENC + 1                                              COUNT    22
C                                                                      COUNT    23
      CALL RGAS(PROOTZ,R2,A2,H2,T2,S1,R,G,NTEST,S,NGAS)                COUNT    24
```

Appendix F (Continued)


```
      PROOTY=HTMV2-H2                                                   COUNT    25
C                                                                       COUNT    26
C                    END OF EQUATION FOR ROOT                           COUNT    27
 112  PROOT(I578) = PROOTY                                              COUNT    28
C                                                                       COUNT    29
 104  IF(NROOT) 102,101,125                                             COUNT    30
 101  NROOT= -1                                                         COUNT    31
      GO TO 103                                                         COUNT    32
 108  ZROOT =ZROOTH                                                     COUNT    33
      PROOT(1)=PROOTX/ZROOT                                             COUNT    34
      GO TO 103                                                         COUNT    35
 107  IF(NF.EQ.1) GO TO 127                                             COUNT    36
      NF = NF- 2                                                        COUNT    37
      IF (NF .LT. 1) NF=1                                               COUNT    38
      PROOT(1) =  PROOT(2)                                              COUNT    39
      NFCHK = NF                                                        COUNT    40
      GO TO 100                                                         COUNT    41
 127  DROOT=(PROOT(2)-PROOT(1))/3.                                      COUNT    42
      PROOT(3)=PROOT(1)+DROOT                                           COUNT    43
      PROOT(4)=PROOT(3)+DROOT                                           COUNT    44
      PROOTZ=PROOT(3)                                                   COUNT    45
      MROOT = 0                                                         COUNT    46
      NROOT=1                                                           COUNT    47
      I578 = 7                                                          COUNT    48
      GO TO 114                                                         COUNT    49
 125  IF(MROOT)131,113,115                                              COUNT    50
 113  PROOTZ=PROOT(4)                                                   COUNT    51
C     PROOT(7)=PROOTY                                                   COUNT    52
      MROOT = 1                                                         COUNT    53
      I578 = 8                                                          COUNT    54
      GO TO 114                                                         COUNT    55
 102  IF (SIGN(PROOT(6),PROOT(5))-PROOT(6)) 107,106,107                 COUNT    56
 106  IF (ABS(PROOT(5)) - ABS(PROOT(6)))103,103,108                     COUNT    57
 103  IF(PROOT(5))124,105,124                                           COUNT    58
 105  PROOT(10)=PROOT(1)                                                COUNT    59
      GO TO 110                                                         COUNT    60
 124  PROOT(2)=PROOT(1)                                                 COUNT    61
      PROOT(6)=PROOT(5)                                                 COUNT    62
      NF=1                                                              COUNT    63
      IF (NROOT1 .EQ.2) NF=NFSAV                                        COUNT    64
 100  CONTINUE                                                          COUNT    65
 131  WRITE (6,111) PROOT(1), PROOT(2), PROOT(5), PROOT(                COUNT    66
     16),PROOTX                                                         COUNT    67
 111  FORMAT(13H0 ER ISENCP1=E14.6,4H P2=E14.6,4H P5=E14.6,4H P6=E14.6,4 COUNT    68
     1H PG=E14.6)                                                       COUNT    69
      CALL ODD(9)                                                       COUNT    70
C     PROOT(8)=PROOTY                                                   COUNT    71
 115  CALL NTERP(1,1,PROOT)                                             COUNT    72
      IF (NFSAV .GT. 1) GO TO  250                                      COUNT    73
      IF(NROOT1 .LE.LIM) GO TO 250                                      COUNT    74
      NFSAV=NROOT1 - LIM1                                               COUNT    75
C     PRINT 225, NFSAV                                                  COUNT    76
 225  FORMAT ( * NEW LIMIT NF=* I4)                                     COUNT    77
      GO TO 250                                                         COUNT    78
 220  IF (NFSAV .GT. NFCHK) GO TO 240                                   COUNT    79
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Appendix F (Continued)

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SUBROUTINE  ISENC                          CDC 6600 FTN V3.0-V34A OPT=1  03/10/75  11.37.59.      PAGE      3
                IF (NROOT1-LIMP1)248,248,235                                          COUNT      80
            235 NF=NFSAV                                                              COUNT      81
                NFSAV =  (NROOT1 -LIMP1) +  NFSAV                                     COUNT      82
          C     PRINT 238, NF, NFSAV                                                  COUNT      83
            238 FORMAT ( * INCREASE LIMIT FROM* I4 * TO*I4)                           COUNT      84
                GO TO 250                                                             COUNT      85
            248 IF (NROOT1 .GT. LIM1) GO TO 250                                       COUNT      86
                NFCHK = NFSAV-1                                                       COUNT      87
            240 NFSAV = NFCHK                                                         COUNT      88
            250 CONTINUE                                                              COUNT      89
           110  PROOTX=PROOT(10)                                                      ISENC      90
          C                                                                           ISENC      91
          C                 PROOTX FINAL VALUE OF ROOT                                ISENC      92
          C                                                                           ISENC      93
                P2=PROOTX                                                             ISENC      94
            5   RETURN                                                                ISENC      95
                END                                                                   ISENC      96
```

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