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**R2D2 — A FORTRAN PROGRAM FOR  
TWO-DIMENSIONAL CHEMICALLY REACTING,  
HYPERHERMAL, INTERNAL FLOWS**

**Volume II — User Guide**

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JANUARY 1980

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Final Report for period May 1978 — September 1979

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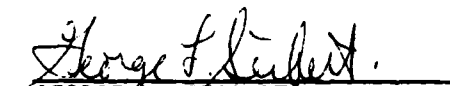
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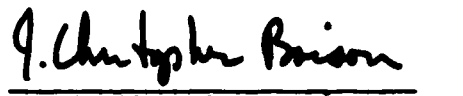
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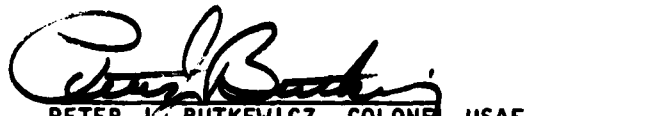
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This technical report has been reviewed and is approved for publication.

  
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→ program dimensions are also presented.

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FOREWORD

The work reported herein was conducted by General Applied Science Laboratories, Inc., principally under contract F33615-78-C-3016 issued by the U.S. Air Force, Air Force Systems Command, Air Force Wright Aeronautical Laboratories, Air Force Flight Dynamics Laboratory, Wright-Patterson AFB, Ohio 45433, under the technical direction of Dr. George Seibert, AFWAL/FIME. The work was also partially supported by GASL internal funds.

The report consists of two parts. The first volume describes the theoretical formulation and method of analysis employed in the subject computer program. The second volume is a guide to the use of the program.

The cooperation of Dr. John Lordi of CALSPAN Corporation in furnishing a listing of their one-dimensional, nonequilibrium streamtube program and related reports is gratefully acknowledged. Portions of the CALSPAN code have been incorporated as subroutines of the subject program, thereby providing a degree of commonality with other nonequilibrium flow programs in current use in the Thermomechanics Branch of the Air Force Flight Dynamics Laboratory.

The work was performed during the period 15 May 1978 to 30 October 1979.

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## LIST OF SYMBOLS

A	$\partial\eta/\partial x_1$
B	$\partial\xi/\partial x_1$
C	$\partial\eta/\partial x_2$
D	$\partial\xi/\partial x_2$
f	index of the last species which is not in vibrational nonequilibrium
g	index of the last species which is in vibrational nonequilibrium
M	Mach number
$MW_\infty$	Molecular weight of mixture at reference or plenum conditions
p	pressure
r	radial coordinate in a cylindrical system
$R_0$	universal gas content
$R_\infty$	gas constant at reference or plenum conditions; $R_0/MW_\infty$
s	number of species
S	entropy
t	time
T	temperature
$Tv_i$	vibrational temperature of $i^{\text{th}}$ species
$u_1, u_2, u_3$	velocity components in $x_1, x_2, x_3$ direction
$v_z, v_r, v_\theta$	velocity components in $z, r, \theta$ direction
$v_x, v_y$	velocity component in $x, y$ direction
$x, y$	Cartesian coordinates
z	axial coordinate in a cylindrical system
$\alpha$	angle between $u_2$ and $u_1$ velocity components

$\beta$	angle between $u_3$ and $u_1$ velocity components
$\gamma_e$	isentropic exponent (equilibrium flow)
$\gamma_f$	ratio of specific heats (frozen flow)
$\zeta$	axial component of vorticity
$\eta$	azimuthal component of vorticity. Also transformed normal coordinate
$\theta$	azimuthal coordinate in a cylindrical system
$\xi$	radial component of vorticity. Also transformed streamwise coordinate
$\rho$	density

## INTRODUCTION

The Fortran Program R2D2 is designed to carry out a finite difference solution of the unsteady equations of motion for an inviscid chemically reacting and/or vibrationally excited mixture of gases, in a two-dimensional (planar or axisymmetric) duct. The program is written in Fortran IV for use on a CDC 6600 computer operating under NOS. Two versions of R2D2 have been developed: one for nonequilibrium chemistry and/or vibrational relaxation, R2D2NE, and the other for fully equilibrated chemistry and vibrational excitation, R2D2EQ. The present version of R2D2NE requires 256K (octal) words of core storage, and R2D2EQ requires 154K (octal). An additional 56K (octal) words are required to compile the source codes. The FTN compiler at OPT=1 has been used for the test cases, although a more efficient executable code may result from use of OPT=2. However, in the authors experience, some caution must be exercised with OPT=2, due to occasional compiler errors.

The present report describes the input and output formats of the programs, the operational procedures, a synopsis of the Main Program, principal subroutines and utility subroutines, examples of the output, and related information pertinent to the use of the program.

## GENERAL DESCRIPTION

### 1. INPUT DATA REQUIREMENTS

The required information which must normally be provided as input data consists of:

- a. Duct geometry
- b. Boundary conditions (inlet/exit stations)
- c. Initial conditions
- d. Finite-difference grid specifications
- e. Output format options

The duct geometry is defined by a series of arbitrarily spaced coordinates along the outer wall, (RTIP, ZTIP), and along the inner wall, axis or plane of symmetry (RHUB, ZHUB). (Note that the Fortran names generally refer to a cylindrical coordinate system, i.e.,  $z=x_1$ ,  $r=x_2$ ,  $v_z=u_1$ ,  $v_r=u_2$ ,  $v_\theta=u_3$ , etc. However, in planar cases, they relate to a Cartesian system, e.g.,  $z=x$ ,  $r=y$ ,  $v_z=v_x$ ,  $v_r=v_y$ ,  $v_\theta=0$ , etc.) The inlet and exit planes, as well as a series of planes which define the boundaries of computational domains into which the duct may be divided, are defined by pairs of axial coordinates ZBDH and ZBDT representing the intersection points of each plane with the duct walls. This data is shown schematically in Figure (1).

The boundary conditions consist of certain combinations of flow properties at the inlet and exit stations, as described in Volume I of this report. These may be given at a series of arbitrarily spaced radial positions along the inlet and exit planes, given by RIN and ROUT, respectively. Since the specified values at these positions will be interpolated and/or extrapolated to the inlet and exit grid points, the first and last values of RIN and ROUT need not lie on the duct walls or axis. See Figure (2).

The data to be specified at the inlet consists of (a) either total pressure, PTINLI, and total temperature, TTINLI, or static pressure, PINLEI, and static temperature, TINLEI, (b) either radial velocity, VRINI, or radial flow angle, ALFAI, or ratio of circumferential vorticity component to density, WETAI, and (c) either circumferential velocity, VTHINI, or circumferential flow angle, BETAI,

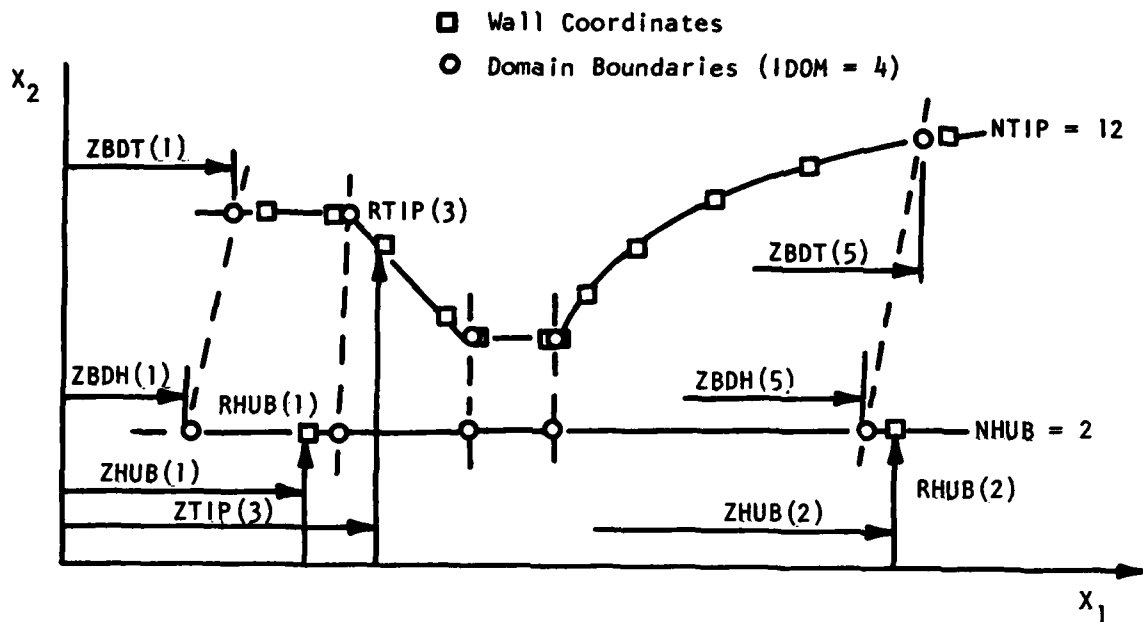


FIGURE 1. SCHEMATIC OF A DUCT SHOWING WALL COORDINATE DATA AND COMPUTATIONAL DOMAIN BOUNDARY DATA.

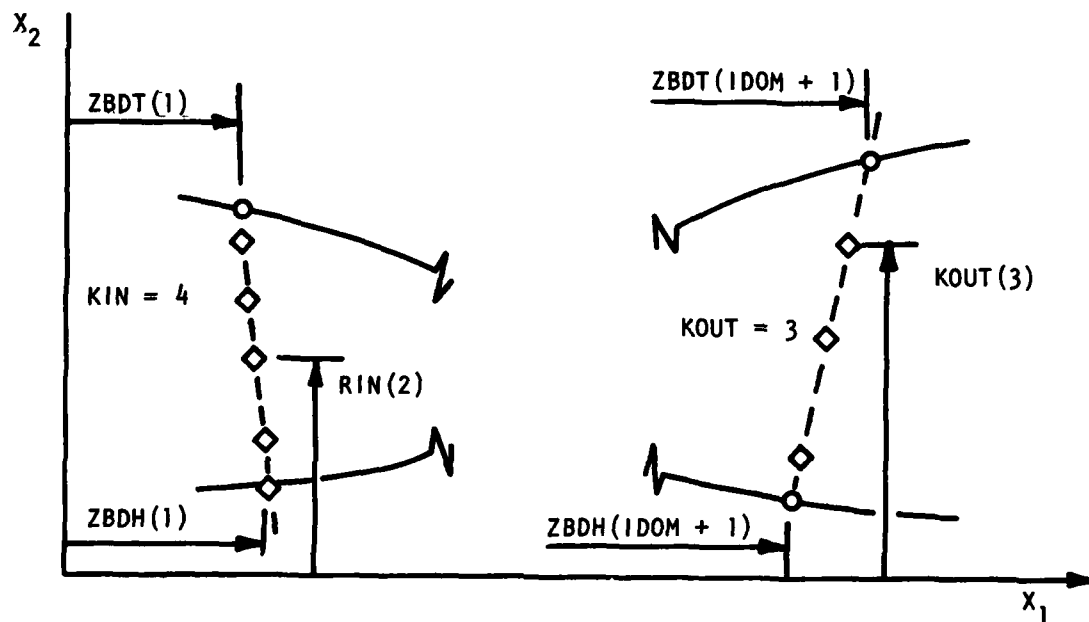


FIGURE 2. DESCRIPTION OF INLET AND EXIT PLANES OF A DUCT AND COORDINATES OF POINTS AT WHICH BOUNDARY CONDITIONS ARE GIVEN.

or ratios of circumferential and axial vorticity components to density,  $WXII$  and  $WZETA I$ . The inlet axial velocity component  $VZINI$  is also specified, however it is only used if the local Mach number is supersonic. At the exit boundary either the total pressure,  $PT\bar{O}UT I$  or the static pressure,  $P\bar{O}UT I$  may be specified. If the exit axial velocity is supersonic, the pressure boundary condition will be automatically replaced by a solution of second characteristic compatibility relation. Although use of the total pressure as the exit boundary condition is admissible, it has been found to be unstable and is therefore not recommended.

In addition, the species concentrations  $ALPHA I$  are specified at the inlet for the nonequilibrium version,  $R2D2NE$ . In the equilibrium version,  $R2D2EQ$ , the values of  $ALPHA I$  denote elemental concentrations.

The initial conditions are obtained in the manner described in Volume I of this report using a specified reference or plenum total pressure,  $PTINF$ , total temperature,  $TTINF$ , and Mach number,  $EMINF$ . A corresponding static pressure,  $PINF$ , temperature,  $TINF$ , and sound speed,  $AINF$ , are computed from the specified reference or plenum data, and used to nondimensionalize all flow variables used within the main body of the program. A reference length  $REF$  is also used to nondimensionalize all lengths.

The finite difference grid is defined by selecting the number of grid columns,  $JMAX$ , and grid rows,  $KMAX$ , for each domain. The domains extend from the lower wall or axis to the upper wall, and from (a) inlet station to the boundary plane of the first domain designated by  $ZBDH(2)$  and  $ZBDT(2)$ ; (b) from there ( $ZBDH(2)$ ,  $ZBDT(2)$ ) to the next boundary plane ( $ZBDH(3)$ ,  $ZBDT(3)$ ); (c) etc., to the exit plane, which terminates the last domain. In general, a domain extends from the boundary plane through ( $ZBDH(I)$ ,  $ZBDT(I)$ ) to the boundary plane through ( $ZBDH(I+1)$ ,  $ZBDT(I+1)$ ). The total number of domains is specified by  $IDOM$ .

The normal output format consists of tabulations of flow properties at each grid point, at selected time intervals; this output format is arranged by grid columns. Provisions for output along specified stations and along specified streamlines is also included in the program, but the associated

coding for printout of the thermochemical data has not been completed.

The data which defines the chemical components of the mixture of gases, their thermodynamic properties and, in R2D2NE, their chemical reaction kinetics, chemical rate constants and vibrational relaxation rates, are contained in a Block Data Subroutine. In R2D2EQ the chemical and vibration rate data are replaced by equilibrium composition data. The present version of R2D2NE includes data for an 8 species, 10 reaction model of high temperature air, taken directly from References (1-3). Consideration of other chemical systems will require recoding of the Block Data Subroutine, and corresponding reidentification of the species labels in the input and output. If the system includes more than 8 species or more than 10 reactions, corresponding increases in the dimensions of certain variables will also be required. In view of the large size of the present version of R2D2NE, the dimensions have been kept at the minimum needed for the air model.

It is also pointed out that the equilibrium version, R2D2EQ, employs the same species model of air as defined in R2D2NE. It has been assumed that the equilibrium concentrations of the 8 species are only a function of pressure and temperature, which implies that the elemental fractions are constant. This would be true for a uniform distribution of the elements across the inlet station. However, if the elements were nonuniformly distributed across the inlet, then the elemental fractions would differ from streamline to streamline. In this case the equilibrium data would have to include the elemental fractions as parameters. In view of this possibility, R2D2EQ includes the solution of species conservations equations for the elemental concentrations. The current version is restricted to a binary system of elements, which are, as noted above, irrelevant to the equilibrium concentrations of species in the assumed model.

Careful attention should be paid to the system of units for the input data. All input (except the Block Data information) is nondimensionalized in Subroutine INDATA, and all output data is consistently redimensionalized in Subroutine OUTPUT. Thus, any self-consistent set of units, e.g., SI, conventional English, CGS, etc., can be used, subject only to the restriction that it must also be consistent with the units used for the thermochemical

data in the Block Data Subroutine. The spatial coordinates present an exception, however, since they need only match the units of the length scale REF, with respect to which they are nondimensionalized, and REF may be in any set of units (or may be nondimensional), independently of the other data.

The current version of R2D2 employs Block Data adopted from References (1-3). Therefore, all input data (except the spatial coordinates) must be in the CGS system, e.g., pressure in dynes/cm<sup>2</sup>, temperature in K, velocity in cm/sec, etc.

## 2. PROGRAM OPERATION

Any particular run should proceed through a specified number of time steps, from an initial time count of `ITIME` to a final time count of `ITIMEF`. Determination of whether an asymptotic (steady) solution has been reached at `ITIMEF` must be made by examining the solution at several intermediate time steps preceding `ITIMEF`. Since the number of time steps required to achieve a steady solution may not, in general, be accurately predictable, the capability to restart a run has been provided. The restart option flag `ISTART` designates whether a run is the initial statement of the problem (`ISTART=0`) or a restart of a previous run (`ISTART=1` or `=2`). A restart run with `ISTART=2` represents a virtually uninterrupted continuation of a previous run, with only a redefinition of the initial and final time counters, `ITIME` and `ITIMEF`, and a possible alteration of the output options. A restart run with `ISTART=1` can utilize the previous flow solution with a redefinition of duct geometry and/or boundary conditions.

Magnetic tape or disc files designated `TAPE1` and `TAPE2` are used as the input media for a restart run, and `TAPE3` and `TAPE4` are used as the output media for storage of data at termination of a run for possible subsequent use in a restart run (i.e., `TAPE3` and `TAPE4` are redesignated as `TAPE1` and `TAPE2`). However, these files are not used during the course of a run.

## 3. OUTPUT DATA

The frequency at which output is obtained at the grid points is controlled by the input parameter `IMESH`, the frequency at which streamline output is obtained is controlled by `ISTREP`, and the frequency of station output is controlled by `ISTATP`. Grid point output can be suppressed by setting `IMESH=0`, streamline output can be suppressed by setting `ISTREM=0`, and station output can be suppressed by setting `ISTAT=0`. (The same effect can also be obtained by setting `IMESH`, `ISTREP` or `ISTATP` to a value larger than `ITIMEF`.) The output data is summarized as follows. It should be noted here

that although the ISTREM and ISTAT options have been included in the input, they have not been fully coded in the present versions of R2D2 and their use is discouraged.

The grid point output consists of the values of the three components of velocity, VZ, VR and VTH, the static pressure and static density, P and  $\overline{RH\bar{O}}$ , the static temperature T, and Mach number MACH, the weight flow rate  $\overline{MD\bar{O}T}$  and the entropy  $\overline{ENTR\bar{O}}$ . The second block of output are the species array ALPHA. In the present versions of the program, Block Data Statements define the order of the species as follows:

- 1st column - oxygen atom ( $\bar{O}$ )
- 2nd column - nitrogen atom (N)
- 3rd column - electron ( $e^-$ )
- 4th column - argon (Ar)
- 5th column - oxygen molecule ( $\bar{O}_2$ )
- 6th column - nitrogen molecule ( $N_2$ )
- 7th column - nitricoxide molecule ( $\overline{NO}$ )
- 8th column - nitricoxide ion ( $\overline{NO^+}$ )

The third block of output for the nonequilibrium version consists of the vibrational temperatures for  $O_2$  and  $N_2$ , respectively. In the equilibrium version, R2D2EQ, this block also includes the elemental mass fractions.

The fourth block of output consists of the mixture static enthalpy, ENTH, mixture specific heats (per unit mass) including all vibrational degrees freedom<sup>4</sup>, CPV and CVV, the mixture specific heats (per unit mass) excluding the nonequilibrium vibrational contributions, CP and CV, the ratio of specific heats ( $\gamma_f$ ), GAMF, and the equilibrium isentropic exponent ( $\gamma_e$ ), GAME (in R2D2EQ only).

(It should be noted that, by definition, the specific heats CP and CV will not include the vibrational contributions even as  $T_{v_i} \rightarrow T$ , since the condition  $T_{v_i} = T$  is not explicitly recognized by the program. Thus, as  $T_{v_i} \rightarrow T$  for all i species in the range  $f < i \leq g$ , CPV and CVV acquire the physical significance usually attributed to specific heats at constant pressure and volume, respectively.)

The system of units in which the variables are printed will correspond to that in which the input is stated, except for the last block which has no counterpart in the input data. The static enthalpy ENTH will be in the units of velocity-squared, and the specific heats will be in units corresponding to the species specific heats given in the Block Data Subroutine.

The streamline output (should it be activated) consists of linearly interpolated data from the flow solution at the grid points. The variables printed are the magnitude of the velocity vector,  $V$ , the radial and circumferential flow angles, ALPHA and BETA, the static pressure,  $P$ , static density,  $\rho_0$  and the ratio of the difference between the mixture entropy and the reference or plenum entropy to the gas constant,  $\overline{ENTR_0}$ . ALPHA is defined as the angle between the radial and axial velocity components, and BETA is the angle between the circumferential and axial components. The entropy is defined using input value of  $\gamma$ , and neglecting entropy due to nonequilibrium reactions.

The station output also consists of linearly interpolated data from the flow solution at the grid points. The variables printed are the same set identified above in the streamline outputs.

Sample printouts from both versions of R2D2 are included in the Appendix.

LIST OF INPUT DATA FOR PROGRAM R2D2NE (NONEQUILIBRIUM)

<u>Card No.</u>	<u>Columns</u>	<u>Format</u>	<u>Description</u>
1	1-80	Hollerith	Title card to identify run.
2	1-15	E15.0	TIME-Elapsed time at which to initiate run (sec).
	16-20	I5	ITIME-Elapsed number of time steps at which the run is initiated.
	21-25	I5	ITIMEF-Number of time steps at which the run is terminated.
	26-30	I5	ISTART-Restart control word: 0=initial run; 1=restart using previously stored flow solution, but read input from cards; 2=restart using previously stored flow solution and all input beyond card 10.
3	1-5	I5	JAY-Option for type of coordinate system: 0=Cartesian system (planar); 1=cylindrical system (axisymmetric).
	6-10	I5	IFLP-Option for use of rotating difference operator: 0=no rotation of alternating difference operator; 1=rotation of difference operator (repeats every 4 time steps)
	11-15	I5	IMESH-Printout option flag for grid-point output: 0=deletes printout at all columns; 1=prints flow solution at grid columns selected on card 4.
	16-20	I5	IMESHP-Time step interval at which mesh point data will be printed (when IMESH=1)
	21-25	I5	*INSTREM-Printout option flag for flow solution along streamlines: 0=delete streamline output; 1=print streamline output.
	26-30	I5	*ISTREP-Time step interval at which streamline output is printed.

---

\* It should be noted that these options have not been fully coded for thermo-chemical output in this version of the program, and their use is discouraged.

<u>Card No.</u>	<u>Columns</u>	<u>Format</u>	<u>Description</u>
3	31-35	I5	*ISTAT-Printout option flag for flow solution at axial stations: 0=delete station output; 1=print station output.
	36-40	I5	*ISTAP-Time step interval at which station output is printed.
4	1-50	I1	JPRINT-Print option flag array for each of the J stations in the flow-field: 0 placed in the Jth column of the card deletes the printout for the Jth stations in the grid; 1 placed in the Jth column of the card allows for the printout of the Jth station in the grid.
5	1-5	I5	NSTRM-Number of points to be printed along each streamline (maximum=50) Note: delete card 5 if ISTREM=0.
	6-10	I5	NSL-Number of streamlines to be printed (maximum=11). Note: delete card 5 if ISTREM=0.
6	1-10	E10.0	ZSTRM(I)-Axial coordinate of Ith point along each streamline (I=1,2,3,...NSTRM); units consistent with REF units. Note: delete card 6 if ISTREM=0. (May be continued on additional cards, as necessary.)
	71-80		
7	1-10	E10.0	RMF(I)=Ratio of weight flow rate of Ith streamtube to total weight flow rate through the duct (I=1,2,3,...NSL). e.g. RMF(1)=0.0, RMF(2)=0.1...RMS(NSL)=1.0. Note: delete card 7 if ISTREM=0. (May be continued on additional cards, as necessary.)
	71-80		

\* It should be noted that these options have not been fully coded for thermo-chemical output in this version of the program and their use is discouraged.

<u>Card No.</u>	<u>Columns</u>	<u>Format</u>	<u>Description</u>
8	1-5	I5	NSTAT-Number of axial stations at which station printout is desired (maximum=10). Note: delete card 8 if ISTAT=0.
	6-10	I5	NSTAP-Number of radial points to be included in the station printout (maximum=11). Note: delete card 8 if ISTAT=0.
9	1-10	E10.0	ZSTATH(I)-Axial coordinates of intersection of axis or centerline and Ith printout station (I=1,2,3...NSTAT); units consistent with REF units. Note: delete card 9 if ISTAT=0. (May be continued on another card is NSTST>8.)
	71-80		
10	1-10	E10.0	ZSTAT(I)-Axial coordinates of intersection of wall point and Ith printout station (I=1,2,3...NSTAT); units consistent with REF units. Note: delete card 10 if ISTAT=0. (May be continued on another card if NSTAT>8.)
	71-80		

WHEN ISTART=2 ALL THE FOLLOWING CARDS ARE DELETED

11	1-5	I5	IDOM-Number of domains into which the duct is to be divided.
	6-10	I5	JMAX(I)-Number of grid stations in the Ith domain (I=1,2,3...IDOM)
	11-15	I5	KMAX(I)-Number of radial grid points in the Ith domain (I=1,2,3...IDOM) (Maximum=21). Note JMAX and KMAX are given in pairs for each value of I=1,...,IDOM. e.g. (JMAX(1), KMAX(1)), (JMAX(2), KMAX(2)). etc.

IDOM  
Note:  $\sum_{I=1}^{IDOM} JMAX(I) \leq 50 - IDOM$  is required.

\* It should be noted that these options have not been fully coded for thermo-chemical output in this version of the program and their use is discouraged.

<u>Card No.</u>	<u>Columns</u>	<u>Format</u>	<u>Description</u>
12	1-5	I5	INOPT-Inlet pressure and temperature option: 0=total pressure and total temperature arrays at the inlet station are specified; 1=static pressure and static temperature arrays are specified; 1=static pressure and static temperature arrays are specified at the inlet.
	6-10	I5	OUTOPT-Discharge pressure option: 0=total pressure array is specified at discharge station*, 1=static pressure array is specified at discharge station.
	11-15	I5	KIN-Number of values to be included in the discharge station input data arrays (maximum=21).
	16-20	I5	KOUT-Number of values to be included in the discharge station input data arrays (maximum=21).
	21-25	I5	IRAD0-Inlet radial velocity component boundary condition option: 0=specify radial velocity component, $v_r$ . (See VRINI on card 22a); 1=specify angle between radial and axial velocity components, $\alpha$ (see ALFAI on card 22b); 2=specify ratio of circumferential component of vorticity to density, $\eta/\rho$ (see WETAI on card 22c).
	26-30	I5	ISWIRL-Inlet circumferential velocity component boundary condition option: 0=specify circumferential velocity component, $v_\theta$ (see VTHNIN on card 23a); 1=specify angle between circumferential and axial velocity components. (See BETAI on card 23b) 2=specify ratios of radial and axial components of vorticity to density $\xi/\rho$ and $\zeta/\rho$ (see WXII and WZETAI on cards 23c and 23d). (This data will be ignored if JAY=0.)

\*OUTOPT=0 is not generally recommended since it has been found to become unstable as the flow approaches a steady state.

<u>Card No.</u>	<u>Columns</u>	<u>Format</u>	<u>Description</u>
13	1-5	I5	NHUB-Number of coordinate points to be specified along lower wall axis or plane of symmetry (maximum=30, minimum=2).
	6-10	I5	NTIP-Number of coordinate points to be specified along the upper wall (maximum=30, minimum=2).
14	1-10	E10.0	GAM-Ratio of specific heats, $\gamma$
	11-20	E10.0	GASCON-Gas constant, $R_{\infty}$ ; dyne cm/gm K
	21-30	E10.0	EMINF-Reference or plenum Mach number
	31-40	E10.0	TTINF-Reference or plenum total pressure; dynes/cm <sup>2</sup>
	41-50	E10.0	PTINF-Reference or plenum total pressure; dynes/cm <sup>2</sup>
	51-60	E10.0	XMDOTF-initial weight flow rate; gms/s
	61-70	E10.0	REF-Nondimensionalizing reference length (arbitrary units)
	71-80	E10.0	MWINF-Reference or plenum molecular weight; grams/mole
15	1-10 . . .	E10.0	ZBDH(I)-Axial coordinates of intersections of boundary planes with lower wall or axis I=1,2,3... (IDOM+1). Units are consistent with REF. (For IDOM=1, I=1 specifies beginning of domain 1, I=2 the beginning of domain 2, and I=3 the end, etc.). May be continued on additional cards if IDOM>8.
	71-80		
16	1-10	E10.0	ZBDT(I)-Axial coordinates of intersections of boundary planes with upper wall of duct, I=1,2... (IDOM+1). Units are consistent with REF. May be continued on additional cards if IDOM>8.

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\*Used only for initialization and definition of entropy in output.

<u>Card No.</u>	<u>Columns</u>	<u>Format</u>	<u>Description</u>
17	1-10 . . . 71-80	E10.0	RIN(I)-Array of radial coordinates of input data points along inlet station (I=1,2,3...KIN); Units consistent with REF. (May be continued on additional cards as necessary.)
18	1-10 . . . 71-80	E10.0	R $\bar{O}$ UT(I)-Array of radial coordinates of input data points along discharge station (I=1,2,3...K $\bar{O}$ UT); Units consistent with REF. (May be continued on additional, as necessary.)
19a	1-10 . . . 71-80	E10.0	PTINL(I)-Inlet total pressure values at RIN(I) (I=1,2,3...KIN), (INOPT=0); dynes/cm <sup>2</sup> . (May be continued as additional cards, as necessary.) Cards 19-23 follow same format.
19b	1-10 . . 71-80	E10.0	PINLETI(I)-Inlet static pressure array (I=1,2,3...KIN), (INOPT=1); dynes/cm <sup>2</sup>
20a	1-10 . . 71-80	E10.0	TTINLI(I)-Inlet total temperature array (I=2,3...KIN). (INOPT=0); <sup>o</sup> K
20b	1-10 . . 71-80	E10.0	TINLEI(I)-Inlet static temperature array (I=1,2,3...KIN). (INOPT=1); <sup>o</sup> K.
21	1-10 . . 71-80	E10.0	VZINI(I)-Inlet Axial velocity component (I=1,2,3...KIN); cm/sec (Only used if local Mach number is subsonic.)

<u>Card No.</u>	<u>Columns</u>	<u>Format</u>	<u>Description</u>
22a	1-10 : 71-80	E10.0	VRINI(I)-Inlet radial velocity component array (I=1,2,3...KIN), (IRAD $\theta$ =0); cm/sec.
22b	1-10 : 71-80	E10.0	ALFAI(I)-Array of inlet flow angle between radial and axial velocity components $\alpha = \tan^{-1}(v_r/v_z)$ , (I=1,2,3...KIN) (IRAD $\theta$ =1); radians
22c	1-10 : 71-80	E10.0	WETAI(I)-Array of ratio of circumferential component of vorticity to density $\eta/\rho$ , at the inlet (I=1,2,3...KIN), (IRAD $\theta$ =2), cm <sup>3</sup> /gm/sec.
23a	1-10 : 71-80	E10.0	VTHINI(I)-Inlet circumferential velocity component array (I=1,2,3...KIN), (ISWIRL=0); cm/sec.
23b	1-10 : 71-80	E10.0	BETAI(I)-Array of inlet flow angle between circumferential and axial velocity components, $\beta = \tan^{-1}(v_\theta/v_z)$ (I=1,2,3...KIN) (ISWIRL=1); radians
23c	1-10 : 71-80	E10.0	WXII(I)-Array or ratio of radial component of vorticity to density $\xi/\rho$ , at the inlet (I=1,2,3...KIN), (ISWIRL=2); cm <sup>3</sup> /gm/sec.
23d	1-10 : 71-80	E10.0	WZETAI(I)-Array of ratio of axial component of vorticity to density, $\zeta/\rho$ , at the inlet (I=1,2,3...KIN). (ISWIRL=2); cm <sup>3</sup> /gm/sec. Note: WZETAI data supplied when ISWIRL=2 only.

<u>Card No.</u>	<u>Columns</u>	<u>Format</u>	<u>Description</u>
24a	1-10 . . . . 71-80	E10.0	PTOUT(I)-Discharge total pressure values at ROUT(I) (I=1,2,3...KOUT). (OUTOPT=0); dynes/cm <sup>2</sup> . (May be continued on additional cards, as necessary.)
24b	1-10 . . 71-80	E10.0	POUTLI(I)-Discharge static pressure array (I=1,2,3...KOUT). (OUTOPT=1); dynes/cm <sup>2</sup>
25	1-10 . . . 71-80	E10.0	TTOUTI(I)-Discharge total temperature array (I=1,2,3...KOUT) (only required for ISWIRL 0) °K. (Not used. Zeros are permissible.)
26	1-10 . . . . 71-80	E10.0	ZH(I)-Axial coordinates along the lower wall axis, or plane of symmetry (I=1,2,3...NHUB). Units consistent with REF. (May be continued on additional cards, as necessary.)
27	1-10 . . . . 71-80	E10.0	RH(I)-Radial coordinates corresponding to axial coordinates ZH given on card 26 above along the lower wall, axis (axisymmetric), or plane of symmetry (two dimensional); units consistent with REF.
28	1-10 . . 71-80	E10.0	ZT(I)-Axial coordinates of upper wall (I=1,2,3...NTIP); units consistent with REF.
29	1-10 . . . 71-80	E10.0	RT(I)-Radial coordinates of upper wall corresponding to axial coordinates ZI given on card 28. (I=1,2,3...NTIP); units consistent with REF.

<u>Card No.</u>	<u>Columns</u>	<u>Format</u>	<u>Description</u>
30	1-10 . . 71-80	E10.0	<p>ALPHAI(I,K)-Array of the I<sup>th</sup> species concentrations in the inlet flow at RIN(K). (K=1,2,3...KIN); moles/gm in the current version of R2D2 the species are input and output in the following order:</p> <p>I=1, OXYGEN ATOM (O)  I=2, NITROGEN ATOM (N)  I=3, ELECTRON (e<sup>-</sup>)  I=4, ARGON ATOM (Ar)  I=5, OXYGEN MOLECULE (O<sub>2</sub>)  I=6, NITROGEN MOLECULE (N<sub>2</sub>)  I=7, NITRICOXIDE MOLECULE (NO)  I=8, NITRICOXIDE ION (NO+)</p> <p>For each species I an array of dimension KIN is read in on a separate set cards. I=1,2,3...8(max).</p>
31a	1-10 : 71-80	E10.0	<p>ALPHAI(9,K)-Array of vibrational temperatures for O<sub>2</sub> in the inlet flow (K=1,2,3...KIN); °K.</p>
31b	1-10 . . 71-80	E10.0	<p>ALPHAI(10,K)-Array of vibrational temperatures for N<sub>2</sub> in the inlet flow (K=1,2,3...KIN); °K.</p> <p>For other chemical systems, the first S values of the ALPHAI(I,K) array (I=1,2,3...S) refer to the molar concentrations, while the next V values (V&lt;2S) refer to the vibrational temperatures.</p>

LIST OF INPUT DATA FOR PROGRAM R2D2EQ (EQUILIBRIUM)

The input for cards 1 through 29 of the equilibrium version of the program is identical to the nonequilibrium input. The following input cards pertain only to the equilibrium program:

<u>Card No.</u>	<u>Columns</u>	<u>Format</u>	<u>Description</u>
30	1-5	15	IVG-Number of element mass fractions to be calculated (maximum=2)
31a	1-10 . . 71-80	E10.0	ALPHAI(1,K)-Array of first element mass fractions in inlet flow at RIN(K) (K=1,2,3...KIN)
31b	1.10	E10.0	ALPHAI(2,K)-Array of second element mass fractions in inlet flow at RIN(K) (K=1,2,3...KIN). If IVG=1, this card is omitted.

## OUTPUT

A sample of the mesh output for the nonequilibrium and the equilibrium versions is contained in the Appendix. Units are given in the CGS system corresponding to the assumed use of CGS units for the input data.

The normal output is broken into the following categories.

- A - Input data
- B - Computed constants
- C - Mesh point output
- D - Streamline output
- E - Station output

### Input Data

The input data cards are printed in card-image format as they are read, with superimposed headings to identify each variable. The information is therefore self-explanatory, and is presented in this manner to facilitate checking for and correcting input errors.

### Computed Constants

- TINF - Reference or plenum static temperature:  $^{\circ}\text{K}$
- PINF - Reference or plenum static pressure;  $\text{dynes}/\text{cm}^2$
- RHINF - Reference or plenum static density;  $\text{gm}/\text{cm}^3$
- AINF - Reference or plenum sound speed;  $\text{cm}/\text{sec}$
- QINF - reference or plenum velocity;  $\text{cm}/\text{sec}$
- K - grid row index
- J - grid column index
- Z - axial distance; units corresponding to REF
- R - radial distance; units corresponding to REF
- A,B,C,D - Components of Jacobian of transformation from  $(z,r)$  to  $(\xi,\eta)$

### Mesh Point Output\*

- Z - Axial distance; units of REF
- R - Radial distance; units of REF
- VZ - Axial velocity component; cm/sec
- VR - Radial velocity component; cm/sec
- VTH - Circumferential velocity component; cm/sec
- P - Static pressure; dynes/cm<sup>3</sup>
- RHO - Static density; gm/cm<sup>3</sup>
- T - Static temperature °K
- MACH - Mach number
- MDOT - Weight flow rate,  $\int_{r_H}^R \rho v_z + \rho v_r D/B) \pi r dr$  evaluated at

$\xi$  = constant; gm/sec

ENTRO - Entropy,  $\Delta S/R_0 = (\log(p/p_\infty) - \gamma \log(\rho/\rho_\infty))/(\gamma-1)$

Block 2 of the mesh point output contains the species concentrations in moles per unit mass, in the following order:

- Oxygen atom (O)
- Nitrogen atom (N)
- Electron (e)
- Argon atom (Ar)
- Oxygen molecule (O<sub>2</sub>)
- Nitrogen molecule (N<sub>2</sub>)
- Nitricoxide molecule (NO)
- Nitricoxide ion (NO<sup>+</sup>)

Block 3 of the mesh point output of the nonequilibrium version contains the vibrational temperatures for O<sub>2</sub> and N<sub>2</sub> in °K. For the equilibrium versions it contains the element mass fractions.

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\*This section will be deleted if IMESH=0

Block 4 of the mesh point output gives the enthalpy  $ENTH(\text{cm}^2/\text{sec}^2)$ , specific heats  $CPV$  and  $CVV(\text{cm}^2/\text{sec}^2 \text{ } ^\circ\text{K})$ ,  $\gamma$ ,  $GAMF$ , and the specific heats  $CP$  and  $CV(\text{cm}^2/\text{sec}^2 \text{ } ^\circ\text{K})$ .

#### Streamline Output \*

- Z - Axial position; units of REF
- R - Radial position; units of REF
- V - Magnitude of the velocity vector; cm/sec
- ALPHA - Angle between the radial and axial velocity components,  
i.e.,  $\alpha = \tan^{-1}(v_r/v_z)$ ; degrees
  
- P - Static pressure; dynes/cm<sup>2</sup>
- RHO - Static density; gm/cm<sup>3</sup>
- ENTRO - Entropy,  $\Delta S/R_0$
- MACH - Mach number

#### Station Output \*\*

The same variables described above in the Streamline Output section are printed in the Station Output.

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\* This section will be deleted if ISTRM=0

\*\* This section will be deleted if ISTAT=0 22

## SYNOPSIS OF MAIN PROGRAM AND SUBROUTINES IN PROGRAM R2D2

A brief discussion of the Main Program, Principal Subroutines, Thermochemical Utility Subroutines and the General Utility Subroutines is given for the Program R2D2. The nonequilibrium and the equilibrium versions of the program differ only in Thermochemical Utility Subroutines, and both versions are included in the discussion thereof.

The Thermochemical Utility Subroutines for the nonequilibrium version and in part for the equilibrium version of R2D2 have been adapted from a one-dimensional, steady, nonequilibrium flow program developed by Calspan (References 1,2,3).

## MAIN PROGRAM

The main program acts in large part as an executive routine which first gathers together the boundary conditions and initial conditions, then advances the solution through the prescribed number of time steps by calling a sequence of subroutines, while also calling a subroutine to print the solution at prescribed time intervals, and then stores the final solution and terminates the run.

A summary of the major elements in the logical construction of the main program are contained in a flow chart presented as Figure (3). The principal computation actually performed in the main program is application of the McCormack finite difference algorithm at the interior points. This operation requires less than 20 statements including separate paths for ITER=1 and 2 and separate DO loops for the fluid mechanical components and the thermochemical components of the system of equations. It is identified in the flow chart simply as "Compute VECT's (predictor solution)" and "Compute V's (corrector solution)." A significant portion of the coding preceding this operation is concerned solely with definition of the rather cumbersome 5<sup>th</sup> component of the H array associated with the temperature forms of the energy equation (see Volume I of this report).

Calculation of a series of fourth-order damping terms is included in the coding of the Main Program. However, the damping terms are multiplied by a coefficient XNU whose value is define by a DATA statement as 0.0. Since this term has not been found to be necessary, it has not been discussed elsewhere in either volume of this report. However, the presence of these terms is pointed out to the user, since they can be activated by redefining the value of XNU in the DATA statement. Values in the range  $0.0 < XNU < 1.0$  may be considered if a need for artificial damping of the solution appears warranted. The terms in question appear only in the momentum and energy equations, and are modeled after the corresponding diffusion and conductivity terms.

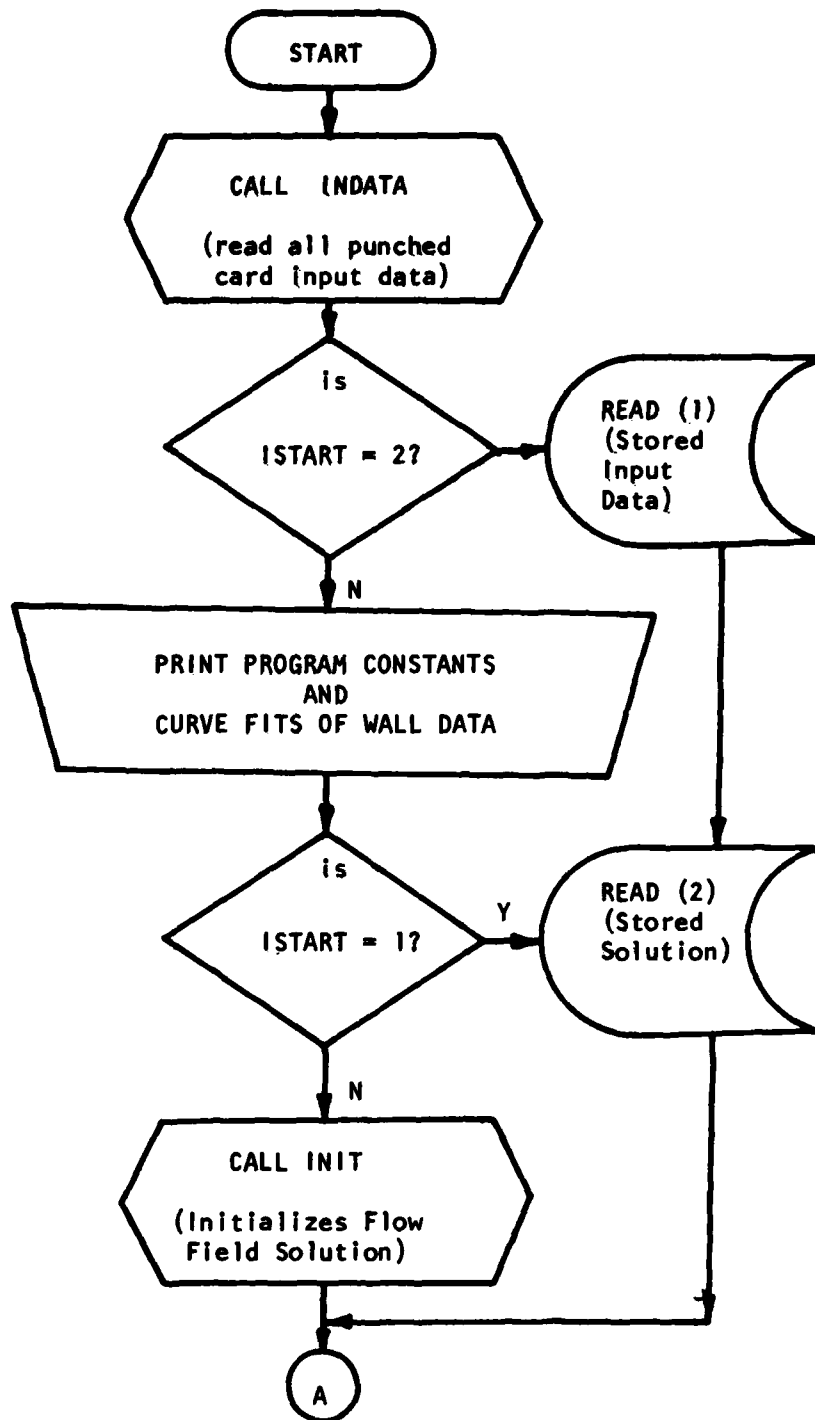


FIGURE 3(a). FLOW CHART OF PROGRAM R2D2  
Part 1 of 4: Initialization.

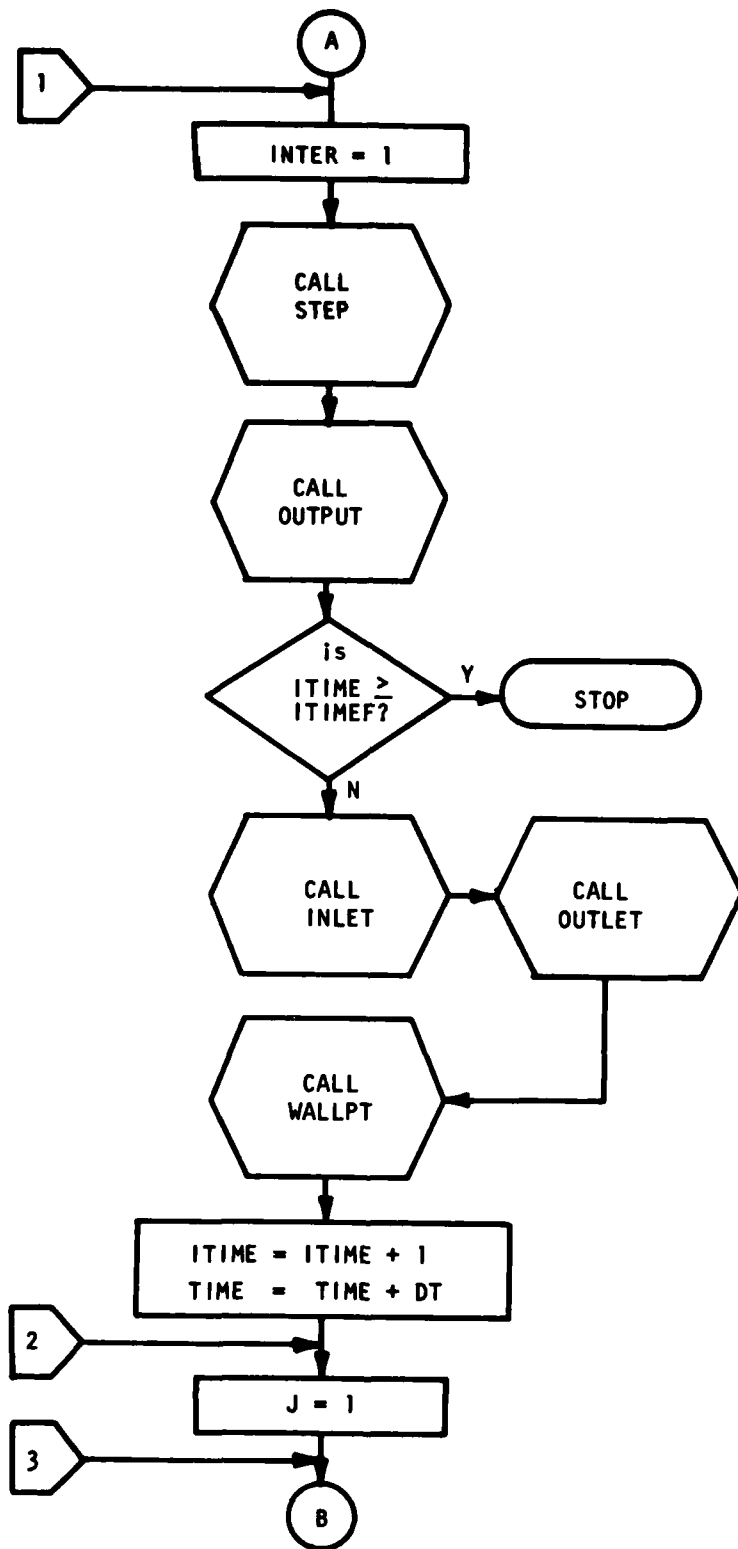


FIGURE 3(b). FLOW CHART OF PROGRAM R2D2  
Part 2 of 4: Start of Time  
Integration Loop.

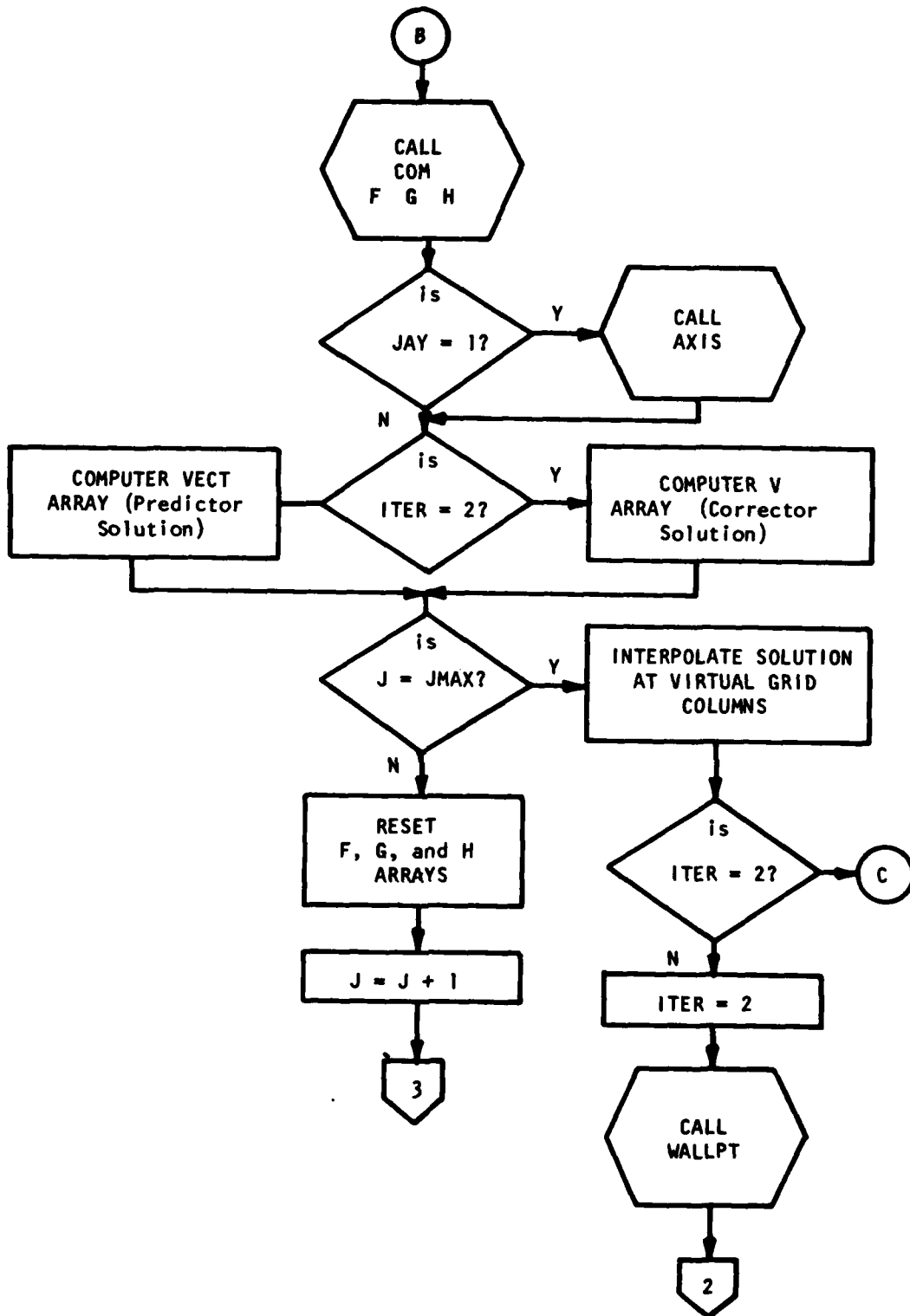


FIGURE 3(c). FLOW CHART OF PROGRAM R202  
Part 3 of 4: Continuation of Time  
Integration Loop.

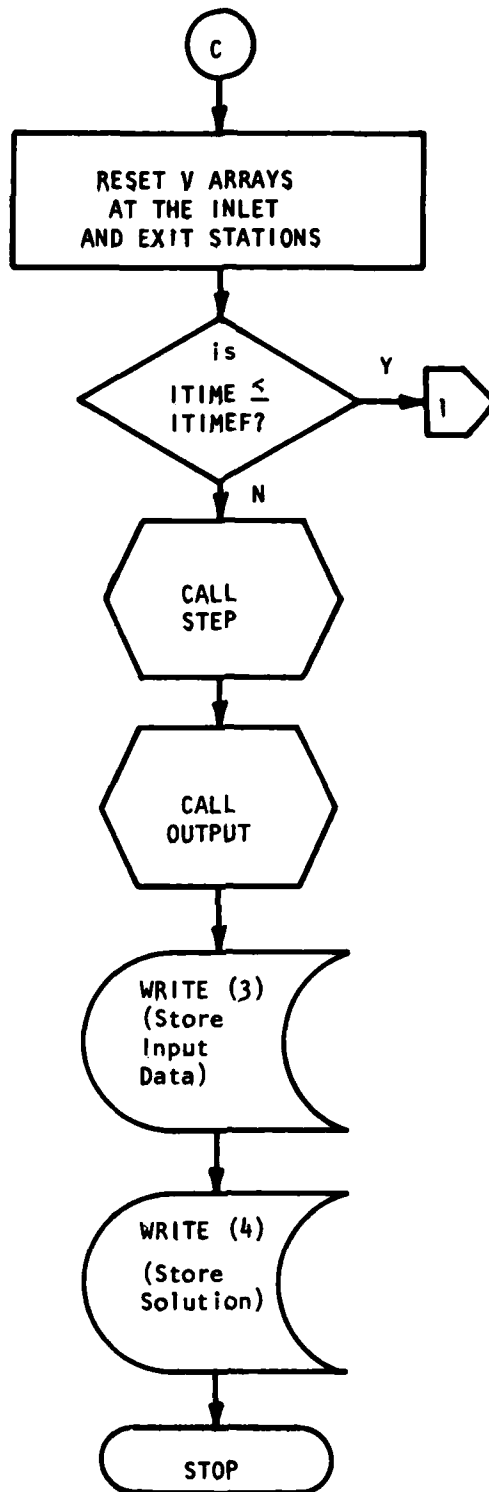


FIGURE 3(d). FLOW CHART OF PROGRAM R2D2  
Part 4 of 4: Termination of Time  
Integration Loop.

## PRINCIPAL SUBROUTINES

### WALLPOINT (ITER,DT)

ITER - iteration index for MacCormack Algorithm (ITER=1 for predictor  
ITER=2 for corrector step)

DT - time step ( $\Delta t_{\omega}/L$ )

Performs the time integration of the governing equations along the duct walls, by a modified version of the interior point finite difference algorithm, excluding wall points at the inlet and outlet stations.

### INLET(DT)

DT - time step ( $\Delta t_{\omega}/L$ )

Imposes the inlet boundary conditions and performs the time integration of the equations at the grid points spanning the inlet station.

### OUTLET(DT)

DT - time step ( $\Delta t_{\omega}/L$ )

Imposes the outlet boundary conditions (if the local Mach number is subsonic) and performs the time integration of the equations at the grid points spanning the outlet station.

### COMFGH(R,N,J,K,JAY,IFLOP,J1)

R - radius array ( $r/L$ )

N - domain index

J - column index

K - row index

JAY - indicator for axisymmetric (JAY=1) or planar flow (JAY=0)

IFLOP - flag signaling end of domain (IFLOP=1 at interior columns, IFLOP=0 at first and last columns of each domain).

J1 - special column index: J1=2 for column at which solution is being advanced, J1=1 for column behind it and J1=3 for column ahead of it. (If  $J < 3$ ,  $J1=J$ )

## INDATA

1. reads all (punched card) input data
2. nondimensionalizes the variables
3. sets up finite difference grid (calls MESH)
4. interpolates inlet and outlet boundary conditions arrays to grid points on inlet and outlet

## INIT

Initializes the flowfield by iterating on a value of temperature (or equivalently pressure) at each grid column that yields a velocity which conserves mass, using a constant total pressure, PTINF, total temperature, TTINF, and mass flow rate XMDOTF. The angular velocity component initializes using conservation of angular momentum along grid rows, which are reasonable approximations to streamlines. The remaining components of velocity are determined by linearly distributing the radial flow angle between the angles at the upper and lower walls (or axis) at that grid column. Species concentrations and vibrational energies are assumed to remain frozen along grid rows (i.e., streamlines).

Note that this initialization procedure only uses the following inlet boundary values: the angular velocity component, the species concentrations, and the vibrational energies. Thus, the remaining boundary conditions are imposed impulsively at the first time step. The values of PTINF and TTINF should be selected judiciously to avoid imposing an extreme impulse on the first step.

Subroutine INIT also calls QIJDOT to initialize the chemical and vibrational time constants for subsequent use in determining the permissible time step.

## OUTPUT(V,V4)

V - three dimensional array of fluid mechanical variables representing the solution at the current time step.

V4 - three-dimensional array of chemical concentrations and vibrational energies representing the solution at the current time step.

The subroutine prints the solution at the specified time intervals. The dependent variable arrays, V and V4, are decoded into primitive variables via a call to GETOUT.

#### COMFGH

Computes the F,G and H arrays corresponding to the generic form of the governing equations:

$$\frac{\partial e}{\partial t} + \frac{\partial f}{\partial x} + \frac{\partial g}{\partial y} = h$$

The E array is defined in the Main Program and transferred through Common Block /I/. The E,F, G and H arrays are triply-dimensioned. The first index refers to the variable, e.g., 1 for  $\rho$ , 2 for  $\rho v_z$ , etc. The second refers to the column, J1. The third refers to the row, K.

COMFGH is called from the Main Program in a loop which results in definition of E,F,G and H arrays at J1=1,2 and 3 initially, and thereafter only at J1=3, in each domain. These arrays at J1=1 and 2 are redefined in the Main Program after completion of the time integration for each column by transferring the J1=2 column to J1=1 and J1=3 to J1=2.

Arrays E4, F4, G4 and H4 contain the chemical species and vibrational energy variables, whereas E,F,G and H contain the fluid mechanical variables.

#### AXIS(ITER, J,N,P,DT)

ITER - iteration index  
J - column index  
N - domain index  
P - pressure array  
DT - time step ( $\Delta t_{\infty}/L$ )

Performs the time integration of the governing equations along an axis of symmetry.

### STEP(DT)

DT - time step ( $\Delta t_{\text{max}}/L$ )

Determines the maximum permissible size of the time step based on current data.

### STREAM(K, J, DT, SDUM, VRDUM, RVPDUM, DVRDT)

K - grid row index

J - grid column index

SDUM - interpolated entropy

VRDUM - interpolated radial velocity component

RVPDUM - interpolated product of angular velocity component and radius

DVRDT - interpolated time derivative of radial velocity component

Performs a stream-path trace from a grid point on the outlet boundary to a point on the (z,r) or (x,y) plane at the previous time step. Variables used in integration of Lagrangian form of the equations are obtained by linear interpolation. May also be called from INLET if the axial velocity component becomes negative at a point on the inlet station.

### MESH(IDOM, ZBDH, ZBDT)

IDOM - number of computational domains

ZBDH - array of locations of intersections of domain boundary stations with the lower wall (or axis). Number of values should be (IDOM+1).

ZBDT - array of Z locations of intersections of domain boundary stations with upper wall. (IDOM+1 values)

Generates a non-orthogonal grid which spans each domain with a specified number of grid columns and rows. The first and last columns are coincident with the domain boundary stations, and interior columns are equally spaced between them. The first and last rows are coincident with the lower wall (or axis) and the upper wall, and the interior rows are equally spaced between them.

The output from MESH is the R(J,K) and Z(J,K) arrays defining the grid point coordinates, the arrays of the first derivatives, DRHDZ and DRTDZ, of the lower and upper walls, respectively, and the Jacobian coefficient matrices, A,B,C

and D, which define the transformation from (Z,R) or (X,Y) to computation coordinates ( $\xi, \eta$ ).

GETOUT(J, K, DUM, VR, VPHE, VZ, P1, RHO1, T1, XMACH, P, RHO, ENTRO, V, V4, ENTH)

J - grid column index  
K - grid row index  
DUM - dummy variable (not used)  
VR - radial component of velocity (dimensional)  
VPHE - angular " " " "  
VZ - axial " " " "  
P1 - static pressure (dimensional)  
RHO1 - static density (dimensional)  
T1 - static temperature (dimensional)  
XMACH - Mach number (frozen sound speed)  
P - nondimensional pressure  
RHO - " density  
ENTRO - " entropy  
V - array of fluid mechanical variables  
V4 - array of chemical concentration and vibrational energy variables  
ENTH - mixture static enthalpy (dimensional)

Decodes the V and V4 arrays into primitive, dimensional variables.

MASSFL(DOTM, I, VV1, VV2, VV3, VV5, VV5)

DOTM - dimensionalizing factor for mass flow rate;  $L^2 \rho_\infty / a_\infty$   
I - column index  
VV1 - array of interpolated values of  $\rho$  at DOTM  
VV2 - array of interpolated values of  $\rho v_z$  at DOTM  
VV3 - array of interpolated values of  $\rho v_r$  at DOTM  
VV4 - array of interpolated values of  $\rho v_\theta r$  at DOTM  
VV5 - array of interpolated values of  $\rho T$  at DOTM

Traces a series of 20 streamlines, or lines of constant mass flow ration in an unsteady flow, and interpolates the solution from the grid points to points along these streamlines.

## THERMOCHEMICAL UTILITY SUBROUTINES

### SPHEAT (W, ALPHA, CP, CV)

- W - temperature ( $T/T_\infty$ )
- ALPHA - species concentrations ( $\gamma_i MW_\infty$ )
- CP - specific heat at constant pressure ( $C_p/R_0$ )
- CV - specific heat at constant volume ( $C_v/R_0$ )

Calculates specific heats (excluding the vibrational energy partition function for those species specified as being in vibrational non-equilibrium). (Adapted from Reference 1.)

### ENTHAL (W, A1, A2, DH, DE, ENI)

- W - temperature ( $T/T_\infty$ )
- A1 - species concentrations ( $\gamma_i MW_\infty$ )
- A2 - vibrational energies ( $e_{v_i}/RoT_\infty$ )
- DH - mixture enthalpy ( $hMW_\infty/RoT_\infty$ )
- DE - mixture internal energy ( $eMW_\infty/RoT_\infty$ )
- ENI - species internal energies ( $e_i/ToT_\infty$ )

Calculates the mixture enthalpy and internal energy, h and e. Also returns with the species internal energies,  $e_{v_i}$ . (The vibrational energy partition function is excluded from the calculation for those species specified as being in vibrational non-equilibrium.) (Adapted from Reference 1.)

QIJDOT (W, P, R, V, A1, A2, QIJ, WEVD)

- W - temperature ( $T/T_\infty$ )
- P - pressure ( $p/p_\infty$ )
- R - density ( $\rho/\rho_\infty$ )
- V - velocity ( $V/a_\infty$ )
- A1 - species concentration ( $\gamma_i MW_\infty$ )
- A2 - species vibration energies ( $e_{v_i}/RoT_\infty$ )
- QIJ - time rate of production of  $i^{\text{th}}$  species due to all chemical reactions
- WEVD - time rate of vibrational relaxation of  $i^{\text{th}}$  species

Calculates the chemical rate of production of species, excluding the group from  $i=1$  to  $e$  which are calculated from conservation of elements. Also calculates the rate of vibrational relaxation for species in the range from  $i=f+1$  to  $g$ , which are assumed to be in vibrational relaxation. Also calculates time constants for chemical and vibrational processes to be used in stability calculation. (Adapted from Reference 1.)

WSUM (IS, IE, DELS, QIJ, WDSUM)

- I - total number of chemical species
- IE - total number of elements ( $IE \leq I$ )
- DELS - coefficient matrix for expressing WDSUM in terms of QIJ
- QIJ - chemical rate of production of species in the range  $i=IE+1$  to  $IS$
- WDSUM - chemical rate of production of species in the range  $i=1, IE$

MOLWT (ALPHA, EMM)

- ALPHA - species concentrations ( $\gamma_i MW_\infty$ )
- EMM - mixture molecular weight ( $MW/MW_\infty$ )

calculates the mixture molecular weight.

GET DEL (IS, IE, DELE, DELS)

- IS - number of chemical species
- IE - number of chemical elements
- DELE - two dimensional square array of numbers of atoms of  $i^{\text{th}}$  element in the  $j^{\text{th}}$  species for species 1,2,3,...IE
- DELS - two dimensional array of numbers of atoms of  $i^{\text{th}}$  element in the  $j^{\text{th}}$  species for species IE+1, IE+2,...IS.

Calculates the coefficient matrix DELS used to relate the rate of production of species  $i=1$  to IE to that for species IE+1 to IS using conservation of elements.

SUBROUTINE SUB6 (I, AIT)

- I - species being handled ( $I=1$ , species is  $\bar{0}$ , etc.)
- AIT - temperature ( $T/T_{\infty}$ )

Computes the electronic excitation contributions to enthalpy, specific heat and chemical potential to the  $I^{\text{th}}$  species (Adapted from Reference 1).

## GENERAL UTILITY SUBROUTINES

### MTRXIN (A,N)

A - matrix of dimension N

N - size of matrix

Inverts the A matrix and returns with  $A^{-1}$  in the same location.

### INI1 (RT, DUM, KMAX, ANS, R)

RT - radial position at which value is to be interpolated

DUM - one-dimensional array of values of variable to be interpolated

KMAX - number of values in DUM array

ANS - interpolated value

R - one-dimensional array of radial coordinates corresponding to the DUM array.

Performs a linear interpolation on a one-dimensional array, and returns with the interpolated value ANS.

### INT (RT, J, DUM, KMAX, ANS, R)

Same as INT1 except R array is two-dimensional, with J as the value of the first index and the second index corresponding to the one-dimensional DUM array.

### INT2 (RT, J, KMAX, R, RAT, IL, IU)

RT - radial position at which interpolation is to be performed

J - value of first index of R array

KMAX - maximum value of the second index of the R array

R - a two-dimensional array of radial positions; the first index is the column and the second is the row.

RAT - ratio of distance from R(J,IL) to RT to distance from R(J,IL) to R(J,IU)

IL - index of row below the position RT

IU - index of row above the position RT

Finds the indices of the rows of the R array, at column J, bounding the radial position RT, and the ratio of distances needed to perform an interpolation.

SPLINE (X, Y, N, EM, SB, G)

- X - array of N coordinates of the set (X,Y)
- Y - array of N coordinates of the set (X,Y)
- N - number of points in the X and Y arrays
- EM - array of second derivatives of spline curve  $d^2Y/dX^2$  at each point
- SB,G - arrays of parameters from spline curve (not needed for further use)

SPLINT (X, Y, N, Z, MAX, YINT, DYDX, DY2DX, EM)

- X - array of N coordinates of the set (X,Y)
- Y - array of N coordinates of the set (X,Y)
- N - number of points in the X and Y arrays
- Z - array of X values at which the spline curve is to be evaluated
- MAX - number of values in the Z, YINT, DYDX and DY2DX arrays
- YINT - array values of Y at X=Z
- DYDX - array of values of first derivative  $DY/DX$  at X=Z
- DY2DX - array of values of second derivative  $d^2Y/dX^2$  at X=Z
- EM - array of second derivatives at the coordinate points (X,Y)

Subroutines SPLINE and SPLINT work in sequence as follows. SPLINE fits a cubic spline curve ( $Y=f(X)$ ) through the given coordinate points (X,Y) and returns with the second derivative  $EM=d^2Y/dX^2$  at the given coordinate points. SPLINT may then be called repeatedly to utilize the spline curve to interpolate values and derivatives of  $Y=f(X)$  at various points. The arrays X,Y in the calling sequences of both subroutines should be identical, although in principle, a subset of (X,Y) can be used in SPLINT. The EM array is output from SPLINE and input to SPLINT. the Z array is input to SPLINT and the YINT, DYDX and DY2DX arrays are output. (Adapted from Reference 5.).

LININT (X, Y, Z, NX, NY, NDIMX, NDIMY, XO, YO, ZO, I, J)

- X - two-dimensional array of X coordinates
- Y - two-dimensional array of Y coordinates
- Z - two-dimensional array of any function of (X,Y)
- NX - initial guess of column index ( $NX \geq 2$ ) for search
- NY - initial guess of row index ( $NY \geq 2$ ) for search
- NDIMX - maximum value of first index of X,Y and Z arrays
- NDIMY - maximum value of second index of X,Y and Z arrays
- XO - X coordinate of point to be interpolated
- YO - Y coordinate of point to be interpolated
- ZO - linearly interpolated value of Z at  $X=XO$  and  $Y=YO$
- I - column index at which search terminates
- J - row index at which search terminates

Performs a general, two-dimensional, linear interpolation of any function  $Z=f(X,Y)$ . The coordinates (X,Y) need not be orthogonal; any four sets of points should, however, form a quadrilateral. The search begins at indices (NX,NY) and ends at (I,J). Therefore repeated calls to LININT to interpolate from one coordinate system to another, for example, should use  $NX=I$  and  $NY=J$ . (From Reference 5.)

The equilibrium version of R2D2, namely R2D2EQ, utilizes the same principal subroutines and general utility subroutines. The thermochemical utility subroutines have been changed to calculate the equilibrium chemical kinetics as prescribed by typical charts for equilibrium air chemistry.

The following are Equilibrium Thermochemical Subroutines. The only difference for subroutines SPHEAT, ENTHAL, and SUB6 between the equilibrium and non-equilibrium packages is that the vibrational temperature in the equilibrium package is set equal to the static temperature.

The following subroutines pertain to R2D2EQ only-

SPHEAT (W, P, ALPHA, CP, CV)

- W - temperature ( $T/T_\infty$ )
- P - pressure ( $P/P_\infty$ )
- ALPHA - species concentrations ( $\gamma_i M_{i\infty}$ )
- CP - specific heat at constant pressure ( $C_p/R_0$ )
- CV - specific heat at constant volume ( $C_v/R_0$ )

Calculates specific heats

ENTHAL(W, P, A1, A2, DH, DE, ENI)

- W - temperature ( $T/T_\infty$ )
- P - pressure ( $P/P_\infty$ )
- A1 - species concentrations ( $\gamma_i M_{i\infty}$ )
- A2 - dummy array
- DH - mixture enthalpy ( $hM_\infty/R_0 T_\infty$ )
- DE - dummy variable
- ENI - dummy array

Calculates the mixture enthalpy

MOLWT (P, T, SUM)

P - pressure ( $P/P_{\infty}$ )

T - temperature ( $T/T_{\infty}$ )

SUM - mixture molecular weight ( $MW/MW_{\infty}$ )

Calculates the equilibrium mixture molecular weight by double interpolation of curve fits of the molecular weight vs temperature for values of pressure.

GAMMA (P, T, GAM)

P - pressure ( $P/P_{\infty}$ )

T - temperature ( $T/T_{\infty}$ )

GAM - equilibrium value of  $\gamma$ .

Calculates the equilibrium  $\gamma$  by a double interpolation of curve fits of gamma vs the temperature for values of pressure.

EQUIL (P, T, ALPHA)

P - pressure ( $P/P_{\infty}$ )

T - temperature ( $T/T_{\infty}$ )

ALPHA - species concentration ( $\gamma_i MW_{\infty}$ )

Calculates the species concentrations by a double interpolation of curve fits for each species. The species are curve fit vs the enthalpy for values of pressure. The enthalpy is obtained from a double interpolation of the curve fits of the enthalpy vs temperature for values of pressure.

CHANGES IN THERMOCHEMICAL DATA AND/OR PROGRAM DIMENSIONS

The chemical kinetics and thermodynamic properties of the system of reacting and vibrationally relaxing gases are fully defined in the BLOCK DATA NE Subroutine of Program R2D2NE. As mentioned previously, the present set of data in this subroutine are taken from the 8 species, 10 reaction model of high temperature air used in References (1-3). The Fortran names are also largely synonymous with those used in References (1-3), since the thermochemical subroutines employ portions of code from the CALSPAN Normal Shock Program described therein. The block data is defined in the following dictionary.

Dictionary of Variables in BLOCK DATA NE

<u>Name</u>	<u>Dimension</u>	<u>Definition</u>	<u>Present Value</u>
IV	-	Number of chemical species	8
IVB	-	Number of elements	4
IF, IG	-	Indices defining range of species in vibrational nonequilibrium (Note: IF=f+1, IG=g)	5,6
IVP, IVBP	-	IV+1 and IVB+1	9,5
THETA(I), THEVJP(I)	8	Characteristic vibrational temperature for ith species	See listing
ETAJ(I)	8	Number of atoms per molecule	4*1.0, 4*2.0
SBJ(I)	8	Constants for chemical potentials	See listing
SHJOP(I)	8	Heats of formation of each species	See listing
CNJ(I)	8	Number of vibrational levels for each species	See listing
CXEF(I)	8	Dummy array (not used - See Reference 1)	See listing
TAUAI(I), TAURJ(I), TAUCJ(I), TAUDJ(I)	8	Constants which describe the vibrational relaxation rate constant for species in the range f+1 < i ≤ g	See listing
MSUMJ(I)	8	Number of electronic levels for each species (maximum of 8 per species)	See listing

SGJL(I,J)	8,8	Degeneracy of $i^{\text{th}}$ electronic level of $j^{\text{th}}$ species	See listing
CEJLPX(I,J)	8,8	Energy of $i^{\text{th}}$ electronic level of $j^{\text{th}}$ species	See listing
TFC(I,J,K)	5,8,2	Dummy array (not used)	80*0
CWI(I), CZI(I), CDI(I)	10	Factors, either 0.0 or 1.0, that control which of 3 forms of the $Q_{ij}$ relationship is used for each reaction	See listing
XNUIJP(I,J)	8,10	Stoichiometric product coefficients for $j^{\text{th}}$ species in $i^{\text{th}}$ reaction	See listing
XNUIJ(I,J)	8,10	Stoichiometric reactant coefficients for $j^{\text{th}}$ species in $i^{\text{th}}$ reaction	See listing
CAIJ(I,J)	8,10	Indices identifying vibration-dissociation coupling for $j^{\text{th}}$ species in $i^{\text{th}}$ reaction	80*0
KFIIND(I)	10	Indicator that denotes direction of the $i^{\text{th}}$ reaction corresponding to the specified rate constants: 0 for forward, 1 for backward	See listing
AKFI(I), BKFI(I), CKFI(I), DKFI(I)	10	Rate constants for $i^{\text{th}}$ chemical reaction: $k = A_i T^{B_i} \exp(-C_i/T^{D_i})$	See listing
EMMLWT(I)	8	Molecular weights of each species	See listing
DELE(I,J)	4,4	Molecular weight of $i^{\text{th}}$ element in the $j^{\text{th}}$ species for first IVB species	See listing
DELS(I,J)	4,8	Molecular weight of $i^{\text{th}}$ element in the $j^{\text{th}}$ species for species IVBP to IV	See listing
CRO	-	Universal gas constant	1,98645
ISR	-	Number of reactions	10
ISS	-	Number of species (same as IV)	8

ISF,ISG	-	f,g (same as IF-1,IG)	4,6
ISC	-	Number of elements (same as IVB)	4
INDSUM	-	Indicator for inclusion of electronic excitation (0-exclude, 1-include)	1
IISFP1	-	f+1 (same as IF and ISFPI)	5
IISF, IISG	-	Same ISF, ISG	4,6
ISCP1	-	ISC+1 (same as IVBP)	5
ISFP1,ISGP1	-	f+1 and g+1	5,7
M	-	s+g-f+3 (where s=IV)	13
M1	-	M+1	14
MX1	-	M-2	
MX2	-	M-1	12
MX3	-	M	13
MX4	-	M+1	14
IDELXC	-	Dummy variable (not used)	0
XNUI(I)	10	Dummy array (not used)	10*0
BBTAI(I)	10	Dummy array (not used)	10*0
EECHJ(I) EECNUJ(I), EECCPJ(I),	8	Dummy arrays (not used)	3*10*0

There are obviously a number of redundancies in the above list of variables, which accrued during the merger of the CALSPAN routines with a nonreacting version of the GASL duct flow program. These could easily be eliminated by judicious use of Equivalence Statements. Superfluous data such as M, M1, MX2, MX3 and MX4 could also be calculated, e.g., from MX1. The dummy arrays have been retained because they are, or may have been, used for temporary storage in the thermochemical subroutines, or are used under options no longer available.

The dimension of 8 in the thermochemical data refers to the number of species, 10 to the number of reactions, and 4 to the number of elements. These dimensions may be increased to accommodate larger systems, if necessary, by changing their values in the COMMON blocks which appear in the BLOCK DATA Subroutine. In addition, if the number of species is increased the dimensions of the dependent variable arrays which contain the species concentrations and vibrational temperatures, e.g., V4, VECT4, ALPHA, etc., must be correspondingly increased. Since every species could, in principle, be a diatomic or polyatomic molecule having its own nonequilibrium vibrational temperature, these dependent variable arrays are dimensioned to twice the number of species; 16 in the present system. Virtually every subroutine would have to be examined for changes in the dimensioned variables in this case.

In some computations, it may become necessary to increase the maximum grid density, which is presently limited to 50 columns and 21 rows. These dimensions appear in virtually all the dependent variable arrays as well as the grid coordinate arrays. Note that the program storage requirement and execution time will escalate quickly with increases in grid density.

Should it be desirable to alter the number of points at which duct wall coordinates are specified, the dimension of 30 identifies the variables and dimensions which will be affected. Similarly, 10 identifies the variables and dimensions associated with station output and 11 identifies streamline output variables and dimensions. The maximum number of points which may be printed along each streamline is currently identical to the maximum number of grid columns, 50, and the maximum number of points at which inlet and exit boundary conditions can be specified is identical to the maximum number of grid rows, 21. This correspondence in dimensions is coincidental, and need not be maintained.

The dimension of 5 appearing in certain variables refers to the number of fluid mechanical equations (continuity, 3 components of momentum, and energy) and should therefore never be altered. The dimension of 3 refers to the use of 3 grid columns in the finite-difference algorithm, and is also therefore invariant. Similarly the dimension of 2 in variables in Subroutine WALLPT refers to the use of 2 grid rows along the walls of the duct, and in

Subroutines INLET and OUTLET to the use of 2 grid columns along the inlet and outlet planes.

With the above guidelines in mind, altering the program dimensions is a straightforward but tedious task.

Program R2D2EQ is virtually the same as R2D2NE except for the replacement of rate expressions by equilibrium thermochemical properties. The data contained in the BLOCK DATA A Subroutine of R2D2EQ is a subset of that described in the previous dictionary. However, additional block data is also defined in Subroutines EQUIL, GAMMA and MOLWT, which utilize cubic spline fits of tabular equilibrium data. These subroutines have been tailored, to a certain extent, to the considered air model. However, their function is clear, and they can be easily recoded for a more general model or for other specific models. For example, the concentrations of components of the 8 species air model, the mixture molecular weight and the isentropic exponent were made available (in graphic form) to the authors as a function of mixture enthalpy and pressure. In addition, the mixture enthalpy was available as a function of pressure and temperature. (This is not the usual format in which such information is obtained but in this case it represented a readily available equilibrium solution which was consistent with the nonequilibrium model.) Therefore, the procedure employed in these subroutines is to first find the enthalpy at the given pressure and temperature, and then find the concentrations, molecular weight and isentropic exponent at that pressure and enthalpy. Obviously, the enthalpy is simply an intermediate variable in determining these properties as a function of pressure and temperature. Thus, its units are irrelevant, and it could be eliminated altogether if the data were supplied in a different form. Furthermore, these subroutines use the fact that one of the species, Argon, is inert and therefore its mass fraction is a constant, and that two of the species,  $\text{NO}^+$  and  $\text{e}^-$ , must have identical mole fractions (to conserve charge). Therefore, tabular data is only supplied for 6 (rather than 8) species.

The data in Subroutines EQUIL, GAMMA and MOLWT is identified by comment statements within each subroutine. However, it is reiterated here that there are 20 entries in the temperature table at each of 3 pressures, or a total of

60 values. Thus, the temperature increments in the tables can be different at each pressure. There are a corresponding 60 entries in each of the tables of enthalpy, molecular weight and isentropic exponent, and a corresponding 60 entries in each of 6 species concentrations tables. Since the cubic spline fits can produce negative concentrations under certain conditions, especially when extrapolating, it has been found useful to fit the logarithm of the concentrations rather than the value. An option has been provided for conversion of the data to its logarithms, and to take the antilog of the fitted curve, which is controlled by ISPEC(I)=0 or 1. ISPEC(I) is defined as 1 for all species in a DATA Statement in the present version of EQUIL, which precludes negative concentrations.

Parenthetically, it is also pointed out that Subroutine EQUIL is only used to provide species concentrations for output; it is not called by the Main program to carry out the time integrations of the governing equations. Subroutines MOLWT and GAMMA are called repeatedly from the Main program and other subroutines to define the molecular weight and isentropic exponent at every grid point on every time step. In particular, the pressure must be determined iteratively from the known density and temperature using the equation of state and Subroutine MOLWT. It appears that this process contributes substantially to the execution of time of R2D2EQ. Thus recoding of MOLWT to provide the molecular weight as a function of density and temperature could enhance the speed of R2D2EQ.

APPENDIX

Sample Printouts from R2D2E0 and R2D2NE





COMPUTED INFINITY CONDITIONS

TINF 6.38722E+03 PINF 1.99229E+08 RHINF 9.62075E-03 AINF 1.43831E+05

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PROGRAM CONSTANTS

K	Z	R	A	B	C	D
j = 1						
1	-2.050E-01	0.	0.	5.000E+01	9.760E+01	0.
2	-2.050E-01	1.025E-02	1.150E+01	5.000E+01	3.760E+01	0.
3	-2.050E-01	2.049E-02	2.335E+01	5.000E+01	9.760E+01	0.
4	-2.050E-01	3.074E-02	3.473E+01	5.000E+01	9.760E+01	0.
5	-2.050E-01	4.098E-02	4.531E+01	5.000E+01	9.760E+01	0.
6	-2.050E-01	5.123E-02	5.708E+01	5.000E+01	9.760E+01	0.
7	-2.050E-01	6.148E-02	6.365E+01	5.000E+01	9.760E+01	0.
8	-2.050E-01	7.172E-02	6.164E+01	5.000E+01	9.760E+01	0.
9	-2.050E-01	8.197E-02	9.261E+01	5.000E+01	9.760E+01	0.
j = 2						
1	-1.050E-01	0.	0.	5.000E+01	1.133E+02	0.
2	-1.050E-01	0.339E-03	2.314E+00	5.000E+01	1.133E+02	0.
3	-1.050E-01	1.290E-02	5.020E+00	5.000E+01	1.133E+02	0.
4	-1.050E-01	2.097E-02	0.783E+00	5.000E+01	1.133E+02	0.
5	-1.050E-01	3.035E-02	1.166E+01	5.000E+01	1.133E+02	0.
6	-1.050E-01	4.094E-02	1.457E+01	5.000E+01	1.133E+02	0.
7	-1.050E-01	5.093E-02	1.749E+01	5.000E+01	1.133E+02	0.
8	-1.050E-01	6.032E-02	2.340E+01	5.000E+01	1.133E+02	0.
9	-1.050E-01	7.031E-02	2.331E+01	5.000E+01	1.133E+02	0.
j = 3						
1	-1.050E-01	0.	0.	5.000E+01	1.102E+02	0.
2	-1.050E-01	0.550E-03	4.302E+00	5.000E+01	1.102E+02	0.
3	-1.050E-01	1.632E-02	9.163E+00	5.000E+01	1.102E+02	0.
4	-1.050E-01	2.337E-02	1.374E+01	5.000E+01	1.102E+02	0.
5	-1.050E-01	3.303E-02	1.933E+01	5.000E+01	1.102E+02	0.
6	-1.050E-01	4.229E-02	2.231E+01	5.000E+01	1.102E+02	0.
7	-1.050E-01	5.075E-02	2.749E+01	5.000E+01	1.102E+02	0.
8	-1.050E-01	5.920E-02	3.207E+01	5.000E+01	1.102E+02	0.
9	-1.050E-01	6.766E-02	3.665E+01	5.000E+01	1.102E+02	0.
j = 4						
1	-1.050E-01	0.	0.	5.000E+01	1.332E+02	0.
2	-1.050E-01	7.583E-03	6.325E+00	5.000E+01	1.332E+02	0.
3	-1.050E-01	1.502E-02	1.365E+01	5.000E+01	1.332E+02	0.
4	-1.050E-01	2.253E-02	2.348E+01	5.000E+01	1.332E+02	0.
5	-1.050E-01	3.004E-02	2.731E+01	5.000E+01	1.332E+02	0.
6	-1.050E-01	3.755E-02	3.413E+01	5.000E+01	1.332E+02	0.
7	-1.050E-01	4.506E-02	4.396E+01	5.000E+01	1.332E+02	0.
8	-1.050E-01	5.257E-02	4.778E+01	5.000E+01	1.332E+02	0.
9	-1.050E-01	6.007E-02	5.651E+01	5.000E+01	1.332E+02	0.
j = 5						
1	-1.050E-01	0.	0.	5.000E+01	1.332E+02	0.
2	-1.050E-01	0.020E-03	0.	5.000E+01	1.332E+02	0.
3	-1.050E-01	0.040E-02	0.	5.000E+01	1.332E+02	0.
4	-1.050E-01	0.060E-02	0.	5.000E+01	1.332E+02	0.
5	-1.050E-01	0.080E-02	0.	5.000E+01	1.332E+02	0.
6	-1.050E-01	0.100E-02	0.	5.000E+01	1.332E+02	0.
7	-1.050E-01	0.120E-02	0.	5.000E+01	1.332E+02	0.
8	-1.050E-01	0.140E-02	0.	5.000E+01	1.332E+02	0.
9	-1.050E-01	0.160E-02	0.	5.000E+01	1.332E+02	0.

FIGURE 4 (c). SAMPLE PORTION OF CALCULATED OUTPUT

NUMBER OF STEPS = 0 TIME = 0.

MESH POINT OUTPUT

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DOMAIN = 1

Z	R	VZ	VR	VTH	P	RHD	TEMP	MACH(F)	MDOT	ENTRO(F)
-2.0530E-01	1.0246E-02	2.5003E+04	4.0	0.	2.0137E+08	9.6261E-03	6.3004E+03	1.6022E-01	0.	5.1699E-02
-2.0530E-01	1.0246E-02	9.5310E+03	-9.3567E+02	2.4410E+04	2.0137E+08	9.6261E-03	6.3004E+03	1.6022E-01	3.1207E-02	5.1699E-02
-2.0530E-01	1.0246E-02	0.	0.	3.4219E+04	1.9957E+08	9.5423E-03	6.2343E+03	2.0440E-01	5.2445E-02	5.1699E-02
-2.0530E-01	3.0730E-02	0.	0.	2.9910E+04	2.0107E+08	9.5934E-03	6.3027E+03	1.7092E-01	6.2415E-02	5.1699E-02
-2.0530E-01	1.0246E-02	8.0169E+03	-3.4437E+03	2.5140E+04	2.0137E+08	9.6261E-03	6.3004E+03	1.6022E-01	1.7488E-01	5.1699E-02
-2.0530E-01	3.1223E-02	1.5461E+04	-7.9519E+03	2.0330E+04	2.0137E+08	9.6261E-03	6.3004E+03	1.6022E-01	5.2701E-01	5.1699E-02
-2.0530E-01	3.1475E-02	1.8344E+04	-1.1742E+04	1.5623E+04	2.0137E+08	9.6261E-03	6.3004E+03	1.6022E-01	1.4222E+01	5.1699E-02
-2.0530E-01	7.1721E-02	1.9239E+04	-1.5107E+04	1.6050E+04	2.0137E+08	9.6261E-03	6.3004E+03	1.6022E-01	1.9833E+00	5.1699E-02
-2.0530E-01	9.1957E-02	1.4393E+04	-1.7366E+04	0.0995E+04	2.0137E+08	9.6261E-03	6.3004E+03	1.6022E-01	2.0411E+00	5.1699E-02

ALPHA 3RAY

2.5228E-01	2.4438E-02	1.1203E-04	0.1204E-03	1.0047E-02	5.3637E-01	0.1558E-02	1.0203E-04			
2.5228E-01	2.4438E-02	1.0203E-04	0.1501E-03	1.0047E-02	6.3637E-01	0.1558E-02	1.0203E-04			
2.5228E-01	2.4438E-02	1.0047E-02	0.1501E-03	1.0047E-02	6.3637E-01	0.1558E-02	1.0203E-04			
2.5228E-01	2.4438E-02	1.0047E-02	0.1501E-03	1.0047E-02	6.3637E-01	0.1558E-02	1.0203E-04			
2.5228E-01	2.4438E-02	1.0047E-02	0.1501E-03	1.0047E-02	6.3637E-01	0.1558E-02	1.0203E-04			
2.5228E-01	2.4438E-02	1.0047E-02	0.1501E-03	1.0047E-02	6.3637E-01	0.1558E-02	1.0203E-04			
2.5228E-01	2.4438E-02	1.0047E-02	0.1501E-03	1.0047E-02	6.3637E-01	0.1558E-02	1.0203E-04			
2.5228E-01	2.4438E-02	1.0047E-02	0.1501E-03	1.0047E-02	6.3637E-01	0.1558E-02	1.0203E-04			

FUEL AIR RATIO

1.0301E+00										
1.0301E+00										
1.0301E+00										
1.0301E+00										
1.0301E+00										
1.0301E+00										
1.0301E+00										
1.0301E+00										

ENTH	ZPV	QVV	GAME	CP	ZV	GAME
1.1201E+01	1.3305E+07	9.9794E+06	1.3333E+06	1.3305E+07	9.9794E+06	1.2308E+00
1.1201E+01	1.3305E+07	9.9794E+06	1.3333E+06	1.3305E+07	9.9794E+06	1.2308E+00
1.1201E+01	1.3305E+07	9.9794E+06	1.3333E+06	1.3305E+07	9.9794E+06	1.2308E+00
1.1201E+01	1.3305E+07	9.9794E+06	1.3333E+06	1.3305E+07	9.9794E+06	1.2308E+00
1.1201E+01	1.3305E+07	9.9794E+06	1.3333E+06	1.3305E+07	9.9794E+06	1.2308E+00
1.1201E+01	1.3305E+07	9.9794E+06	1.3333E+06	1.3305E+07	9.9794E+06	1.2308E+00
1.1201E+01	1.3305E+07	9.9794E+06	1.3333E+06	1.3305E+07	9.9794E+06	1.2308E+00
1.1201E+01	1.3305E+07	9.9794E+06	1.3333E+06	1.3305E+07	9.9794E+06	1.2308E+00

FIGURE 4 (d). SAMPLE OF MESH POINT OUTPUT

MACH(F)	MDOT	ENTRO(F)
03 9.7207E-01	0.	9.1162E-02
03 9.7207E-01	2.3670E-01	9.1162E-02
03 9.7207E-01	9.1486E-01	9.1162E-02
03 9.7207E-01	2.0530E+00	9.1162E-02





COMPUTED CAPACITY DEPOSITIONS

TIME OF DEPOSITION 2.20161E+11 2.5110E+11 2.82023E+11 3.12932E+11

COEFFICIENTS

K	Z	J	I	5	6	7
1	1.000E+00	0.	0.	3.00E+00	2.655E+01	0.
2	1.000E+00	1.687E-02	-2.175E+01	3.00E+00	2.655E+01	0.
3	1.000E+00	7.533E-02	-4.370E+01	3.00E+00	2.655E+01	0.
4	1.000E+00	1.130E-01	-6.522E+01	3.00E+00	2.655E+01	0.
5	1.000E+00	1.507E-01	-8.670E+01	3.00E+00	2.655E+01	0.
6	1.000E+00	1.884E-01	-1.081E+02	3.00E+00	2.655E+01	0.
7	1.000E+00	2.261E-01	-1.295E+02	3.00E+00	2.655E+01	0.
8	1.000E+00	2.638E-01	-1.509E+02	3.00E+00	2.655E+01	0.
9	1.000E+00	3.015E-01	-1.723E+02	3.00E+00	2.655E+01	0.
10	1.000E+00	3.392E-01	-1.937E+02	3.00E+00	2.655E+01	0.
11	1.000E+00	3.769E-01	-2.151E+02	3.00E+00	2.655E+01	0.
12	1.000E+00	4.146E-01	-2.365E+02	3.00E+00	2.655E+01	0.
13	1.000E+00	4.523E-01	-2.579E+02	3.00E+00	2.655E+01	0.
14	1.000E+00	4.900E-01	-2.793E+02	3.00E+00	2.655E+01	0.
15	1.000E+00	5.277E-01	-3.007E+02	3.00E+00	2.655E+01	0.
16	1.000E+00	5.654E-01	-3.221E+02	3.00E+00	2.655E+01	0.
17	1.000E+00	6.031E-01	-3.435E+02	3.00E+00	2.655E+01	0.
18	1.000E+00	6.408E-01	-3.649E+02	3.00E+00	2.655E+01	0.

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K	Z	J	I	5	6	7
1	1.263E+00	0.	0.	3.00E+00	2.510E+01	0.
2	1.263E+00	1.431E-02	-2.111E+01	3.00E+00	2.510E+01	0.
3	1.263E+00	2.862E-02	-4.222E+01	3.00E+00	2.510E+01	0.
4	1.263E+00	4.293E-02	-6.333E+01	3.00E+00	2.510E+01	0.
5	1.263E+00	5.724E-02	-8.444E+01	3.00E+00	2.510E+01	0.
6	1.263E+00	7.155E-02	-1.055E+02	3.00E+00	2.510E+01	0.
7	1.263E+00	8.586E-02	-1.266E+02	3.00E+00	2.510E+01	0.
8	1.263E+00	1.001E-01	-1.477E+02	3.00E+00	2.510E+01	0.
9	1.263E+00	1.144E-01	-1.688E+02	3.00E+00	2.510E+01	0.
10	1.263E+00	1.287E-01	-1.899E+02	3.00E+00	2.510E+01	0.
11	1.263E+00	1.430E-01	-2.110E+02	3.00E+00	2.510E+01	0.
12	1.263E+00	1.573E-01	-2.321E+02	3.00E+00	2.510E+01	0.
13	1.263E+00	1.716E-01	-2.532E+02	3.00E+00	2.510E+01	0.
14	1.263E+00	1.859E-01	-2.743E+02	3.00E+00	2.510E+01	0.
15	1.263E+00	2.002E-01	-2.954E+02	3.00E+00	2.510E+01	0.
16	1.263E+00	2.145E-01	-3.165E+02	3.00E+00	2.510E+01	0.
17	1.263E+00	2.288E-01	-3.376E+02	3.00E+00	2.510E+01	0.
18	1.263E+00	2.431E-01	-3.587E+02	3.00E+00	2.510E+01	0.

K	Z	J	I	5	6	7
1	1.526E+00	0.	0.	3.00E+00	2.374E+01	0.
2	1.526E+00	1.703E-02	-2.105E+01	3.00E+00	2.374E+01	0.
3	1.526E+00	3.406E-02	-4.210E+01	3.00E+00	2.374E+01	0.
4	1.526E+00	5.109E-02	-6.315E+01	3.00E+00	2.374E+01	0.
5	1.526E+00	6.812E-02	-8.420E+01	3.00E+00	2.374E+01	0.
6	1.526E+00	8.515E-02	-1.052E+02	3.00E+00	2.374E+01	0.
7	1.526E+00	1.021E-01	-1.262E+02	3.00E+00	2.374E+01	0.
8	1.526E+00	1.191E-01	-1.472E+02	3.00E+00	2.374E+01	0.
9	1.526E+00	1.361E-01	-1.682E+02	3.00E+00	2.374E+01	0.
10	1.526E+00	1.531E-01	-1.892E+02	3.00E+00	2.374E+01	0.
11	1.526E+00	1.701E-01	-2.102E+02	3.00E+00	2.374E+01	0.
12	1.526E+00	1.871E-01	-2.312E+02	3.00E+00	2.374E+01	0.
13	1.526E+00	2.041E-01	-2.522E+02	3.00E+00	2.374E+01	0.
14	1.526E+00	2.211E-01	-2.732E+02	3.00E+00	2.374E+01	0.
15	1.526E+00	2.381E-01	-2.942E+02	3.00E+00	2.374E+01	0.
16	1.526E+00	2.551E-01	-3.152E+02	3.00E+00	2.374E+01	0.
17	1.526E+00	2.721E-01	-3.362E+02	3.00E+00	2.374E+01	0.
18	1.526E+00	2.891E-01	-3.572E+02	3.00E+00	2.374E+01	0.

FIGURE 5 (c). SAMPLE OF CALCULATED OUTPUT FROM R2D2NE

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