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PREMIXING-PREVAPOORIZING FUEL-AIR MIXING
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Analytical Modeling of Operating Characteristics of Premixing-Prevaporizing Fuel-Air Mixing Passages

Vol. II User's Manual

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February 1982

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NASA Lewis Research Center
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| 16. Abstract A model for predicting the distribution of liquid fuel droplets and fuel vapor in premixing-prevaporizing fuel-air mixing passages of the direct injection type is reported herein. This model consists of three computer programs; a calculation of the two-dimensional or axisymmetric air flow field neglecting the effects of fuel; a calculation of the three-dimensional fuel droplet trajectories and evaporation rates in a known, moving air flow; a calculation of fuel vapor diffusing into a moving three-dimensional air flow with source terms dependent on the droplet evaporation rates. The fuel droplets are treated as individual particle classes each satisfying Newton's law, a heat transfer, and a mass transfer equation. This fuel droplet model treats multi-component fuels and incorporates the physics required for the treatment of elastic droplet collisions, droplet shattering, droplet coalescence and droplet wall interactions. The vapor diffusion calculation treats three dimensional, gas-phase, turbulent diffusion processes. The analysis includes a model for the autoignition of the fuel-air mixture based upon the rate of formation of an important intermediate chemical species during the pre-ignition period. This species is produced both within the vicinity of the fuel droplets and throughout the diffusing fuel vapor-air mixture. The model, as represented by these computer codes, is applied to two premixing fuel-air mixing passage designs and the results are discussed. An application of the autoignition model is also presented. | | | |
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Analytical Modeling of Operating Characteristics of
Premixing-Prevaporizing Fuel-Air Mixing Passages

Volume II - User's Manual

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1.0 SUMMARY

A User's Manual describing the operation of three computer codes (ADD code, PTRAK code, and VAPDIF code) is presented herein. This manual is organized for the convenience of the user and contains sections describing the general features of the computer codes, the input/output formats, run streams, and sample input cases. It is presented in loose leaf format so that changes may be made easily as additional capabilities are added to the computer programs.

This User's Manual constitutes Volume II of the final report under NASA Contract NAS3-21269.

2.0 INTRODUCTION

This User's Manual describes the computer codes used to calculate the operating characteristics of premixing-prevaporizing fuel/air mixing passages. The calculation procedure utilizes three computer codes: the ADD code which calculates the axisymmetric or two-dimensional distributions of velocity, pressure, and temperature of the air flow; the PTRAK code which calculates the nonequilibrium heat-up, vaporization, and trajectories of the liquid fuel droplets in a three-dimensional flow field; and the VAPDIF code which calculates the diffusion of fuel vapor or critical autoignition species into a moving air stream. A detailed description of the analytical models and numerical procedures used in these computer codes is given in Volume I. The User's Manual, Volume, II, contains a description of the operation of the computer codes.

The ADD code was originally developed for NASA Lewis Research Center under Contract NAS3-15402 (Ref. 1). Important revisions, including the conformal mapping coordinate generator, were developed for the U. S. Army Air Mobility Research and Development Laboratory under Contract No. DAAJ02-73-C-0037 (Ref. 2). Further development and improvements to the ADD code were funded by United Technologies Research Center and Pratt & Whitney Aircraft, Commercial Products Division. Additional improvements, including the incorporation of a two-equation model of turbulence into the ADD code, was sponsored by NASA Lewis Research Center under Contract NAS3-21853 (Ref. 3). A complete description of the ADD code is given in Ref. 4 together with a new coordinate generator sponsored under contract DEN3-235.

The original version of the PTRAK code was developed by United Technologies Research Center with its own funding. This version was based on a simple equilibrium vaporization model for single-component fuels. The nonequilibrium heat-up and vaporization model for a distillate fuel was developed under the current contract, NAS3-21269.

The VAPDIF code was developed exclusively under the current contract although it is largely based on the Contractor's experience in developing three-dimensional parabolic forward marching computer codes for predicting the behavior of compressible flows.

This User's Manual is organized into several sections for the convenience of the computer code user. Section 3.0 contains a description of the general features of each of the computer codes to provide the user with an overview of the types of problems which can be solved. Sections 4.0, 5.0 and 6.0 contain descriptions of the operation of each of the computer codes. Sections 3.0 through 6.0 should provide the user with sufficient information of setup and solve typical problems within the scope of the computer codes. Sections 7.0, 8.0, 9.0 present a more detailed description of the PTRAK and VAPDIF codes. A description of the ADD code is given in Ref. 4.

This User's Manual constitutes Volume II of the final report under Contract NAS3-21269.

3.0 GENERAL FEATURES

3.1 General Features of ADD Code

Program Language

The Annular Diffuser Deck (ADD) code source program is written in FORTRAN V computer language for use on a UNIVAC 1100/81A computer. Some machine specific language, such as PARAMETER and INCLUDE FORTRAN statements, is used. However, these statements may be replaced easily by equivalent code for use on other machines. Successful conversions of the code to both IBM and CDC computers have been made and these versions of the code are available. The ADD code makes use of a UNIVAC routine NTRAN which stores and retrieves large data blocks on disc files; however, the ADD code is organized so that NTRAN is easily replaced by the equivalent FORTRAN DEFINE FILE. Finally, it should be noted that the ADD code makes use of least squares spline fitting and smoothing subroutines provided by IMSL, Inc. which are available at all major computer centers.

Fluid Properties

The ADD code can treat any compressible fluid with constant thermodynamic properties for the gas constant R and the specific heats Cp and Cv. The molecular viscosity, which is temperature dependent, is estimated using Sutherland's law; the molecular thermal conductivity is calculated using a constant value for Prandtl number. The viscosity of the fluid at standard conditions and Prandtl number are input parameters. If these properties are not specified in the input data, the ADD code uses the properties of air at standard conditions.

Types of Flow That May Be Treated

The ADD code may be used to treat subsonic compressible laminar or turbulent swirling flow in axisymmetric ducts or nonswirling flow in two-dimensional ducts. The duct may be annular or two-dimensional with both inner and outer walls; or, it may be an axisymmetric duct with only an outer wall. Subsonic flows have been treated successfully up to the sonic line. The mixing of hot and cold streams has also been analyzed using the ADD code. The code is not applicable to flows containing regions of separation or reverse flow.

Duct Geometry Option (IØPT3)

The flow through axisymmetric or two-dimensional ducts may be calculated provided that the principal flow direction is axial; however, the duct cannot contain a right-angle turn. The ADD code is not applicable to flows in ducts with discontinuities in flow area that produce regions of flow separation.

For convenience, provision is made in the code to analyze flows in straight annular ducts (IØPT3=1) or in straight wall, annular diffusers (IØPT3=3) using only a few input parameters. For ducts of arbitrary shape (IØPT3=2), the coordinates (radii) of the inner and outer walls are specified at JLPTS equally-spaced axial stations. To assure that the curve representing the duct contour has continuous first and second derivatives, a least-squares spline fitting, smoothing and interpolation procedure is included in the code. This procedure is used whenever the number of streamwise stations (JL) is not equal to JLPTS.

The specification of the duct geometry must include a straight, annular inlet section whose length is at least equal to its height. Two-dimensional ducts are treated as annular ducts in which the height of the duct is small compared to the radius of the duct. Numerical experiments have shown that, if the height of the duct is less than 1/100 of the duct radius, the flow is essentially two-dimensional to an accuracy of three decimal places.

Inlet Flow Options (IØPT1)

Any arbitrary inlet flow conditions may be specified which are consistent with the equations of motion and the turbulence model. Two types of input data are required: (1) specification of the inviscid free stream and core flow conditions, and (2) specification of the laminar or turbulent boundary layer flow parameters. With IØPT1=3, 4, 9, the flow is assumed to be turbulent and with IØPT1=7, 8, the flow is assumed to be laminar. With IØPT1= 3 or 7, the core flow is calculated assuming that the stagnation pressure and stagnation temperature are constant across the duct. The input Mach number and swirl angle determine the velocities and weight flow, and the static pressure is determined by solving the conservation equation for radial momentum. When IOPT1= 4 or 8, the inlet core flow is determined by specifying KLL data points for fractional distance Y, stagnation pressure $P_T(Y)$, static pressure $P(Y)$, swirl angle $\alpha(Y)$, and stagnation temperature $T_T(Y)$. For IØPT1=9, the core flow is determined by specifying KLL data points for fractional distance Y, streamwise velocity $U_S(Y)$, stagnation pressure $P_T(Y)$, swirl velocity $U_\phi(Y)$, and stagnation temperature $T_T(Y)$. Isentropic flow relations and radial momentum conservation equations are used to determine the remaining variables. In addition, when IØPT1=4, 8 or 9, the corresponding exit flow data must be provided. These data are not required by the calculation procedure but are used only by plotting routines which can be used to compare calculated and measured exit flow profiles. If the exit plane data are not available, the inlet plane data may be repeated.

The boundary layer velocity and temperature profiles are constructed from known analytic solutions using the boundary layer displacement thickness (δ^*) and a power law (1/n) velocity profile. For laminar boundary layers (IOPT1=7, 8) a Blasius profile is assumed. For turbulent flows (IOPT1=3, 4, 9), Cole's boundary layer profile is used with the shape parameter determined from 1/n.

In many flow situations, it is often more convenient to specify the weight flow rather than velocity or Mach number. For these situations, the user may specify the weight flow when using IØPT1= 4 or 8. The static pressure profile is automatically adjusted to obtain the required weight flow with the other input variables held fixed.

It should be noted that the initial plane conditions must satisfy the laws of motion and be compatible with the turbulence model. Therefore, the ADD code makes many checks on the input data to assure satisfactory starting conditions. As an example, the initial plane data are checked to determine if the radial momentum conservation equation is satisfied. If it is not satisfied, the input static pressure profile is replaced by the static pressure profile calculated from the radial momentum equation and a DIAGNØSTIC message is printed. The weight flow calculated from the initial plane data is checked to see if it is greater than the choked-flow value. If it is greater, the calculation stops and the value of the choked weight flow is printed out. Checks are made to assure that the boundary layer profile can be matched to the free stream core flow; the necessary adjustments are made automatically and the calculation continues. In all cases where adjustments to the input data are made and the calculation continues, a DIAGNØSTIC message is printed. When no adjustment is possible or when the flow situation is physically impossible, the calculation stops and the user is notified with a DIAGNØSTIC message. A list of these DIAGNØSTIC messages is given in Section 4.4

Grid Selection

The user may determine the calculation grid using input parameters or the grid may be determined automatically. In either case the user must specify the number of streamwise stations (JL) and the number of streamlines (KL). Experience has shown that a 50 x 50 mesh is suitable for most problems. Default options exist for both the distribution of mesh points in the cross flow direction as specified by the mesh distortion parameters DDS and the streamwise step size parameter KDS. In selecting the mesh distortion parameters DDS, numerical accuracy requires that a sufficient number of mesh points exist in the turbulent sublayer. In practice, the first mesh point from the wall should be at $Y^+ = 1.0$ and at least 20 mesh points should be in the boundary layer. These criteria depend on both the flow Reynolds number and wall friction coefficient. Therefore, if DDS is not specified in the input data, a value for DDS is calculated using an algorithm which produces good results for most cases. The value for the streamwise step size parameter KDS depends on the boundary layer thickness and rate of growth of the boundary layer. If KDS is not specified, the code selects a value for KDS between each streamwise station using an algorithm which produces satisfactorily results for most cases.

Print Options (IØPT4)

The frequency and quantity of output are controlled by the print option IØPT4. If IØPT4 > 0, the output consists of the mean flow variables including streamwise

velocity U_s , tangential velocity U_ϕ , static pressure P , stagnation pressure P_T , stagnation temperature T_T , and Mach number M at each streamwise station for JL stations; this printout occurs at every IØPT4th station. If $IØPT4 \leq -1$, additional information is printed including the effective turbulent viscosity and thermal conductivity, the boundary layer solution in universal coordinates $U^+(Y^+)$, and the turbulent kinetic energy distribution; this information is printed every IØPT4th station.

Diagnostics

The ADD code makes numerous checks during the progress of the calculation. If the program is able to remedy a detected problem, a DIAGNØSTIC is printed and the calculation continues. If a fatal error is detected, the calculation stops and a DIAGNØSTIC notifies the user about the nature and location of the error. A complete list of DIAGNØSTICS is given in Section 4.4.

Calculation Option (IØPT9)

The calculation of the coordinate system may be stored on a data file and retrieved for use in subsequent cases. If IØPT9=1, both the coordinates and the viscous flowfield are calculated. If IØPT9=2, the coordinate system is calculated and stored on file NINE and the calculation stops. If IØPT9=3, the coordinates stored on file NINE are recalled and the viscous flowfield is calculated. This feature is particularly useful when the user wishes to calculate several flows using the same duct geometry.

Data Files

Since three separate computer codes are used in the analysis, data is passed from one computer code to the other through data files. The ADD code generates the coordinate system and stores the results on file NINE. The ADD code also generates the viscous flowfield solution and stores the results on file EIGHT. Both the PTRACK and VAPDIF codes require the data stored on files EIGHT and NINE. The PTRAK code calculates the rate of evaporation of fuel droplets for use as the source terms for the solution of the diffusion equation by the VAPDIF code. These source terms are stored on file SEVENTEEN. The VAPDIF code uses the data stored on all three files. It is recommended that these files be registered and catalogued files so that the data may be stored permanently over a period of several weeks. Proper use of these files allows the user great flexibility in solving problems.

Start/Stop Options

A flow calculation may be started at coordinate station $J=IØPT15$ and it may be terminated at coordinate system station $J=IØPT16$. If IØPT15 is not specified, it is assigned a value IØPT15=1; if IØPT16 is not specified, it is assigned a value IØPT16=JL. The calculation of the flowfield may be continued (or restarted) at the JM coordinate station by specifying IØPT17=JM.

Turbulence Models (IØPT12)

The ADD code is provided with four turbulence models described in Volume I. For IØPT12= 0, 1, 2 algebraic turbulence models are used based on Prandtl's mixing length theory. For IØPT12=3, a two equation model of turbulence is used. Option IØPT12=0 uses a turbulence model which is well established for equilibrium turbulent flowfields and is therefore recommended for all calculations. The other options (IØPT12= 1, 2, 3) are operation but these models have been applied to only a few flowfield situations; the use of these models is not recommended at the present time.

Blade Force Options (IØPT2) (IØPT5) (IØPT10)

Struts, inlet guide vanes, stators, and rotors are modeled in the ADD code as a-priori body forces. Three options exist in the code for calculating these forces. If measurements of stagnation pressure P_T , swirl angle α , and stagnation temperature T_T are available, the blade forces can be calculated from blade element theory by setting IØPT2=1. If IØPT5=2, the program uses the inlet/exit flow data for IØPT1=4. If IØPT5=1, separate data must be read for the blade force calculation. If IØPT2=3, the blade force is calculated from the flow conditions and blade geometry using blade element theory and empirical cascade correlations. If IØPT2=4, the blade force is calculated using the distributions of exit air swirl angle $\alpha_2(Y)$ and loss coefficient $Z_B(Y)$.

IØPT10 determines whether the blade is stationary (IØPT10=1, stator) or rotating (IØPT10=2, rotor).

Global Iteration (IØPT14)

The ADD code can treat small regions of separated and reattached flow (a separation bubble) using a global iteration procedure. For these cases, KDS must be specified. The first iteration is made with IØPT14=0. The second and successive iterations are made by repeating the calculation with IØPT14=1. As successive passes (iterations) are made, the solution stored on file EIGHT is updated.

3.2 General Features of PTRAK Code

Program Language

The Particle Tracking (PTRAK) code is written in the FORTRAN V computer language for use on a UNIVAC 1100/81A computer. Some machine specific language, such as PARAMETER and INCLUDE FORTRAN statements, is used. However, these statements may be replaced easily by equivalent code for use on other machines. The PTRAK code makes use of a UNIVAC routine NTRAN which stores and retrieves large data blocks on disc files; the PTRAK code is designed so that NTRAN is easily replaced with the equivalent FORTRAN DEFINE FILE statements by modifying only one subroutine.

Grid Selection

The PTRAK axial and radial coordinates and computational grid are calculated by the ADD code and stored in file NINE. In addition, the PTRAK code uses the viscous flowfield solution generated by the ADD code and stored in file EIGHT. All information required by the PTRAK code, such as number of mesh points (JL x KL), the starting station (JFIRST), and the termination station (JLAST) are also stored on coordinate file NINE. Information on the third (ϕ) coordinate must be input to the PTRAK code. This information consists of the number of azimuthal grid points ($LPHI \leq 50$), and the azimuthal step size ($\Delta\phi$). Finally the number of axial steps per ADD code streamwise station (KDS) must be specified. The appropriate value of KDS is determined primarily by how rapidly both the droplet trajectories and velocities are changing. At the present time, no algorithm to alter the axial step-size automatically exists in the PTRAK code so that KDS must be set to the largest value (smallest step size) required for an accurate solution.

Boundary Conditions (IØPT3)

Two types of boundary conditions are possible: a wall boundary condition or a periodic boundary condition. At a solid wall, a droplet may either strike the wall and remain thereon or it may rebound elastically. Droplets remaining on a wall may undergo additional evaporation. Droplet-solid wall interaction boundary conditions include: elastic rebound with no vaporization (IØPT3=0, 1); elastic rebound with vaporization (IØPT3= 2, 3). A periodic boundary condition is available for swirling flows in annular ducts. Thus if IØPT3= 1 or 3, the duct is assumed to have four rectangular solid walls. If IØPT3= 0 or 2, the duct is assumed to be an annular duct defined by solid walls and two permeable side-walls with periodic boundary conditions such that, if a droplet exits through one side-wall, an identical droplet will enter through the opposite side-wall; therefore, only an annular segment of the flow needs to be analyzed.

Location of Fuel Injectors

Each of several fuel injectors may be placed arbitrarily in the duct at any axial station by specifying its coordinates (r, z, ϕ). The calculation will start at the first computed viscous flowfield station generated by the ADD code. Integration of the droplet equations will not start until the axial station is reached at which the first fuel injector is located; it will continue until all of the fuel droplets have evaporated.

Initial Droplet Conditions

The initial droplet conditions for each class of droplets consist of its three initial velocity components, diameter, and temperature; up to 1250 droplet classes may be input. The PTRAK code uses a forward marching calculation procedure so that all droplet classes must have an initial velocity component in the downstream direction. Injection angles are limited, therefore, to values less than 85 deg relative to the axial direction.

Composition of Fuel Droplets

Droplets of either single component or multicomponent (distillate) fuels may be considered by specifying the appropriate thermodynamic and transport properties described in Section 4.4 of Volume I. For droplets of distillate fuel, it is necessary to provide both a distillation curve and a Cox chart.

Droplet/Droplet Collisions (IØPT1, IØPT2)

Models for droplet shattering (controlled by IØPT1) and droplet-droplet collisions and coalescence (controlled by IØPT2) are available in the program.

Autoignition Model (IØPT7)

Source terms for the rate of production per unit volume of the critical species for autoignition can be calculated for use subsequently in the VAPDIF code.

3.3 General Features of VAPDIF Code

Program Language

The Vapor Diffusion (VAPDIF) code is written in the FORTRAN V computer language for use on a UNIVAC 1100/81A computer. Some machine specific language, such as PARAMETER and INCLUDE FORTRAN statements, is used; however these statements may be replaced easily by the equivalent code for use on other machines. The PTRAK code makes use of a UNIVAC routine NTRAN which stores and retrieves large data blocks on disc files; the PTRAK code is designed so that NTRAN is easily replaced with the equivalent FORTRAN DEFINE FILE statements by modifying only one sub-routine.

Grid Selection

The VAPDIF code uses the coordinates and computational grid generated by the ADD code and stored in file NINE. In addition it uses the viscous flowfield solution generated by the ADD code and stored in file EIGHT together with the vapor and critical species source distributions and boundary conditions generated by the PTRAK code and stored in various files. All information required to locate data at corresponding grid points is stored in these files.

Boundary Conditions

The boundary conditions are specified completely by the ADD code and PTRAK code data files.

Initial Conditions

It is assumed that the initial concentration of fuel vapor is zero. However, the user may specify a constant mass fraction CZERO (card 4) which is distributed uniformly over the entire initial plane.

Restart Option

The calculation may be started, terminated, or restarted at any axial station in the duct. These options are controlled by the input parameters IADD, IBEGIN, and IEND on input card 2. The variable IADD is equal to JFIRST from the ADD code calculation. IBEGIN is the first calculation station, not including the initial plane, for the VAPDIF code. Normally, the calculation is started with IBEGIN equal to IADD + 1. IEND is the last calculation station in terms of the ADD code coordinates. If IBEGIN > IADD + 1, the code assumes that the solution has been calculated and stored in file ELEVEN for station IADD up to station IBEGIN-1. Thus by specifying IBEGIN and IEND the calculation can be started and stopped at any point.

Print Options (IPRNTX)

Since the VAPDIF code solves a three-dimensional problem, very large amounts of data are necessary to describe completely the solution. For a maximum of a 100 streamwise stations, 100 normal (radial), and 50 tangential stations, there are 5×10^5 grid points. At each grid point the concentration (C), the three coordinates (n, s, ϕ), the three metric coefficients, the three physical distances, and the three cartesian coordinates must be specified. Therefore the total number of data points is 6.5×10^6 . Print options (card 3) may be used to limit the data printout. In all cases, however, a summary table is given which includes the fuel vapor flow rate, fuel air ratio, and mass flow weighted average mass fraction of fuel as a function of axial distance.

Autoignition Model

Subsequent to the calculation of the three-dimensional fuel vapor distribution, the Vapor Diffusion code can be used to determine the distribution of critical species and thereby estimate whether autoignition of the fuel vapor-air mixture will occur.

4.0 OPERATION OF THE ADD CODE

4.1 Runstream for ADD Code

It is assumed that:

1. The program will be executed in TPF\$;
2. The executable (absolute) element is MAPADD;
3. A catalogued file exists for storing the viscous flowfield (and is called EIGHT in this example);
4. A catalogued file exists for storing the flowfield geometry (and is called NINE in this example).

Then the following runstream is sufficient to execute the ADD code.

```
@ASG,AX EIGHT.,D/O/TRK/300000
@ASG,AX NINE.,D/O/TRK/250000
@USE 8,EIGHT
@USE 9,NINE
@ASG,T 10,D/O/TRK/6000
@ASG,T 11,D/O/TRK/50000
@ASG,T 14,D/O/TRK/60000
@ASG,T 22,D/O/TRK/300000
@XQT  MAPADD
(INPUT CARDS)
@FREE 8
@FREE 9
@FREE 10
@FREE 11
@FREE 14
@FREE 22
```

4.2 Input Format for ADD Code

The input format for the ADD code is described on the input data coding forms which follow. These coding forms are organized with one form per input data card. Each form contains the names of the variables, the format, and a description of the data. The input option card controls the data that must be read. Since not all cards are read, the user should make certain that the input data agrees with the input options.

In general the input data is read as follows:

- Card 1 Title Card
- Card 2 Option Card
- Card 3 Mesh Parameter Card
- Card 4 Duct Geometry Card
 + data as required by IØPT3
- Card 5 Inlet Flow Card
 + data as required by IØPT1
- Card 6 Force Data Card (If IØPT2 ≠ 0)
 + data as required by IØPT2, IØPT5, IØPT10
- Card 8 Slot Flow Data Card (option not available)

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ADD CODE INPUT

Card 2 OPTION CARD FORMAT (34I2)

| | | |
|----|--------|----|
| 1 | I0PT1 | 75 |
| 2 | I0PT2 | 76 |
| 3 | I0PT3 | 77 |
| 4 | I0PT4 | 78 |
| 5 | I0PT5 | 79 |
| 6 | I0PT6 | 80 |
| 7 | I0PT7 | 81 |
| 8 | I0PT8 | 82 |
| 9 | I0PT9 | 83 |
| 10 | I0PT10 | 84 |
| 11 | I0PT11 | 85 |
| 12 | I0PT12 | 86 |
| 13 | I0PT13 | 87 |
| 14 | I0PT14 | 88 |
| 15 | I0PT15 | 89 |
| 16 | I0PT16 | 90 |
| 17 | I0PT17 | 91 |
| 18 | I0PT18 | 92 |
| 19 | I0PT19 | 93 |
| 20 | I0PT20 | 94 |
| 21 | I0PT21 | 95 |
| 22 | I0PT22 | 96 |
| 23 | I0PT23 | 97 |
| 24 | I0PT24 | 98 |
| 25 | I0PT25 | 99 |
| 26 | I0PT26 | 00 |
| 27 | I0PT27 | 01 |
| 28 | I0PT28 | 02 |
| 29 | I0PT29 | 03 |
| 30 | I0PT30 | 04 |
| 31 | I0PT31 | 05 |
| 32 | I0PT32 | 06 |
| 33 | I0PT33 | 07 |
| 34 | I0PT34 | 08 |
| 35 | I0PT35 | 09 |
| 36 | I0PT36 | 10 |
| 37 | I0PT37 | 11 |
| 38 | I0PT38 | 12 |
| 39 | I0PT39 | 13 |
| 40 | I0PT40 | 14 |
| 41 | I0PT41 | 15 |
| 42 | I0PT42 | 16 |
| 43 | I0PT43 | 17 |
| 44 | I0PT44 | 18 |
| 45 | I0PT45 | 19 |
| 46 | I0PT46 | 20 |
| 47 | I0PT47 | 21 |
| 48 | I0PT48 | 22 |
| 49 | I0PT49 | 23 |
| 50 | I0PT50 | 24 |
| 51 | I0PT51 | 25 |
| 52 | I0PT52 | 26 |
| 53 | I0PT53 | 27 |
| 54 | I0PT54 | 28 |
| 55 | I0PT55 | 29 |
| 56 | I0PT56 | 30 |
| 57 | I0PT57 | 31 |
| 58 | I0PT58 | 32 |
| 59 | I0PT59 | 33 |
| 60 | I0PT60 | 34 |
| 61 | I0PT61 | 35 |
| 62 | I0PT62 | 36 |
| 63 | I0PT63 | 37 |
| 64 | I0PT64 | 38 |
| 65 | I0PT65 | 39 |
| 66 | I0PT66 | 40 |
| 67 | I0PT67 | 41 |
| 68 | I0PT68 | 42 |
| 69 | I0PT69 | 43 |
| 70 | I0PT70 | 44 |
| 71 | I0PT71 | 45 |
| 72 | I0PT72 | 46 |
| 73 | I0PT73 | 47 |
| 74 | I0PT74 | 48 |
| 75 | I0PT75 | 49 |
| 76 | I0PT76 | 50 |
| 77 | I0PT77 | 51 |
| 78 | I0PT78 | 52 |
| 79 | I0PT79 | 53 |
| 80 | I0PT80 | 54 |
| 81 | I0PT81 | 55 |
| 82 | I0PT82 | 56 |
| 83 | I0PT83 | 57 |
| 84 | I0PT84 | 58 |
| 85 | I0PT85 | 59 |
| 86 | I0PT86 | 60 |
| 87 | I0PT87 | 61 |
| 88 | I0PT88 | 62 |
| 89 | I0PT89 | 63 |
| 90 | I0PT90 | 64 |
| 91 | I0PT91 | 65 |
| 92 | I0PT92 | 66 |
| 93 | I0PT93 | 67 |
| 94 | I0PT94 | 68 |
| 95 | I0PT95 | 69 |
| 96 | I0PT96 | 70 |
| 97 | I0PT97 | 71 |
| 98 | I0PT98 | 72 |
| 99 | I0PT99 | 73 |
| 00 | I0PT00 | 74 |

The input option parameters I0PT1 through I0PT17 determine program flow options to be executed by the ADD code and determine the input data cards to be read. These options are described on the following pages.

The input option parameters IDBC1 through IDBC17 are debug options not normally used. These options are described in Sec. 4.5

IØPT1 (FLØWIN Option)

- = 3 Inlet flow is computed by specifying data on Card 5. (turbulent flow)
- = 4 Inlet and exit flow profiles are read from 2*KLL data cards following Card 5. Input, fractional distance Y , stagnation pressure $P_T(Y)$, static pressure $P(Y)$, swirl angle $\alpha(Y)$, and stagnation temperature $T_T(Y)$. (turbulent flow)
- = 7 Inlet flow is computed by specifying data on Card 5 (laminar flow)
- = 8 Same as 4 but for laminar flow .
- = 9 Same as 4 but: Input fractional distance Y , stagnation pressure $P_T(Y)$, streamwise velocity $U_S(Y)$, swirl velocity $U_\phi(Y)$ and stagnation temperature $T_T(Y)$. (turbulent flow)

IØPT2 (FORCE Option)

- = 0 No blade force
- = 1 Calculate blade force from upstream/downstream flow data; input fractional distance Y , stagnation pressure $P_T(Y)$, static pressure $P(Y)$, swirl angle $\alpha(Y)$, and stagnation temperature $T_T(Y)$
- = 2 Not available
- = 3 Calculate blade force from cascade correlations
- = 4 Calculate blade force from fractional distance Y , exit flow swirl angle $\alpha_2(Y)$, and loss coefficient $Z_B(Y)$

IØPT3 (GDUCT Option) Information follows Card 2

- = 1 Calculate a straight, annular duct.
- = 2 Read co-ordinates of duct.
- = 3 Calculate a straight-walled, annular diffuser.

IØPT4 (PRINT Option)

Print solution every IØPT4 station. For example, if IØPT4 = 3, every third station will be printed. If IØPT4 \leq -1, the code provides an extended printout; this extended printout includes information about the boundary layer profiles and the turbulence model.

IØPT5 (STRUT INPUT Option)

Strut input data (if IØPT2 = 1) used to calculate strut forces from experimental data measured upstream and downstream of strut.

- = 1 Read in required profiles.
- = 2 The upstream and downstream strut data cards are identical to the inlet and exit flow cards and are not read.

IØPT6 (STRUT Thickness Effects)

- 0 Include strut forces plus thickness effects
- 1 Include strut thickness effects only.

IØPT7 Not Used

IØPT8 (PLOT Option)

- = 0 No plots requested.
- = 1 Make CALCØMP plots (not available at LeRC)

IØPT9 (COORDINATE Option)

- = 0 Make an approximate calculation for both streamlines and potential lines--do not save flowfield on disk. Used only for IØPT3=1.
- = 1 Make exact calculation of streamlines and potential lines--store results on logical unit 9 and complete viscous flow calculation.
- = 2 Same as 1 but terminate calculation after coordinate calculations are completed.
- = 3 Read geometry from logical unit 9 and use in viscous flow calculation.

IØPT10 (RØTØR Option)

- = 0 No rotors or stators.
- = 1 Stators are present.
- = 2 Rotors are present.

IØPT11 (FLOW Option)

= 0 Internal flow.

= 1 External flow.

IØPT12 (TURBULENCE Option)

= 0 Use two-layer turbulence model.

= 1 Use two-layer turbulence model with low Reynolds number correction.

= 2 Use two-layer turbulence model with streamline curvature correction.

= 3 Use two equation turbulence model (applicable to flows in annular diffusers only; i.e., diffusers with both inner and outer walls).

IØPT13 (SLOT Option) (Not available)

= 0 No slot cooling.

= 1 Slot cooling.

IØPT14 (GLOBAL Option)

= 0 Global iterations not used.

= 1 Global iterations used - backward differencing for streamwise velocity derivatives in vicinity of separation.

IØPT15 (JFIRST Option)

Start flow calculation at station IØPT15--if omitted, IØPT15 = 1.

IØPT16 (JLAST Option)

Stop calculation at station IØPT16--if omitted, IØPT16 = JL.

IØPT17 (RESTART Option)

Restart a previously generated case at station IØPT17.

NOTE: IØPT9 must be equal to 3 and KDS must be the same value as used in previous run (see Card 3).

4.3 Output Description for ADD Code

The output on each page from the ADD code is largely self-explanatory. A general description of the output by page is given below.

Title Page

This page presents a list of modifications, dates, and report numbers for all changes to the ADD code.

Input Data Page

This page presents all input data including all options and default input values.

Inlet Flow Pages

If IØPT1 = 4, 8 or 9, the input data is checked for self-consistency. Both input and derived results are printed on these pages.

Performance Page

Mean and average quantities of the inlet flow which are frequently used to measure or normalize duct performance are printed on this page.

Wall Conditions Page

The coordinates of the hub and tip wall, mass flow bleed, and wall temperature are printed. For adiabatic walls, the wall temperature is not known before the calculation and appears as $T_w = 0$ on the printout.

Wall Geometry Page

This page prints the wall coordinates, wall curvature, and arc length along the walls.

Gap Average Inviscid Flow Pages

The ADD code calculates the inviscid flow field and prints the solution for each streamwise station as determined by the print option IØPT4.

Gap Average Viscous Flow Pages

The ADD code calculates the viscous flow field solution and prints the solution for each streamwise station as determined by the print option IØPT4. The solution appearing on these pages is stored on file EIGHT.

Boundary Layer Coordinate Pages

When $I\emptyset PT4 < 0$, the velocity and shear stress distribution in universal coordinates $U^+(Y^+)$ and $\tau^+(Y^+)$ and the effective turbulent viscosity and thermal conductivity distributions predicted by the turbulence model are printed.

Turbulence Properties Pages

When $I\emptyset PT4 < 0$, the calculated distribution of turbulence kinetic energy, Reynolds stress, Reynolds number of turbulence, and turbulent Richardson number are printed.

Mass Flow Average Page

At the completion of the calculation, a flow summary is given which includes mass flow weighted averages of several variables, pressure recovery coefficient, and pressure loss coefficient.

Wall Surface Conditions Page

This page presents a summary of wall heat transfer conditions including wall friction coefficient, wall temperature, integrated wall area, and integrated heat transfer through the wall.

Wall Radiation Summary Page

This page presents a summary of data required for wall radiation calculations. This output is not applicable for cases in which the ADD code is applied to pre-mixing fuel preparation passages.

Boundary Layer Parameter Pages (Hub and Tip)

These pages summarize the growth of the boundary layer in terms of displacement thickness, momentum thickness, and shape factor.

4.4 Diagnostics for ADD Code

Numerous checks are made during the course of the calculation. If a minor error occurs, a DIAGNOSTIC message is printed and the calculation continues. If a fatal error occurs, a DIAGNOSTIC message is printed and the calculation stops. A description of these DIAGNOSTICS is given in this section. The DIAGNOSTIC message is always of the form:

****DIAGNOSTIC NO. XX FOR ANNULAR DIFFUSER DECK****

where xx refers to one of the errors listed. It should be noted that numerical values printed with the DIAGNOSTIC message will be in dimensionless form or in English units.

1) IØPT3 OUTSIDE RANGE OF ALLOWABLE DUCT OPTIONS

This error is detected in Subroutine ALTMN. The input option must be between $1 \leq IØPT3 \leq 6$.

2) No solution exists in AMFOR

This error is detected in Subroutine AMFOR. This subroutine solves the Mach number function

$$N = M \left(1 + \frac{\gamma - 1}{2}\right)^{\frac{1}{2}} / (1 + \gamma M^2)$$

for M given N. The function has a maximum at $M = 1$. Hence

$$N(1) = [2(1 + \gamma)]^{-\frac{1}{2}}$$

Solutions do not exist for values of $N > N(1)$.

3) MASS FLOW EXCEEDS THE MAXIMUM MASS FLOW POSSIBLE

This error is detected in Subroutine AMINLT which solves the Mach number function

$$N = M \left(1 + \frac{\gamma - 1}{2} M^2\right)^{-\frac{\gamma + 1}{2(\gamma - 1)}}$$

for M given N. This function has a maximum for $M = 1$ given by

$$N(1) = \left(\frac{\gamma + 1}{2}\right)^{-\frac{\gamma + 1}{2(\gamma - 1)}}$$

corresponding to choked flow.

4) ISHAPE AND IØPT2 ARE NOT CONSISTENT

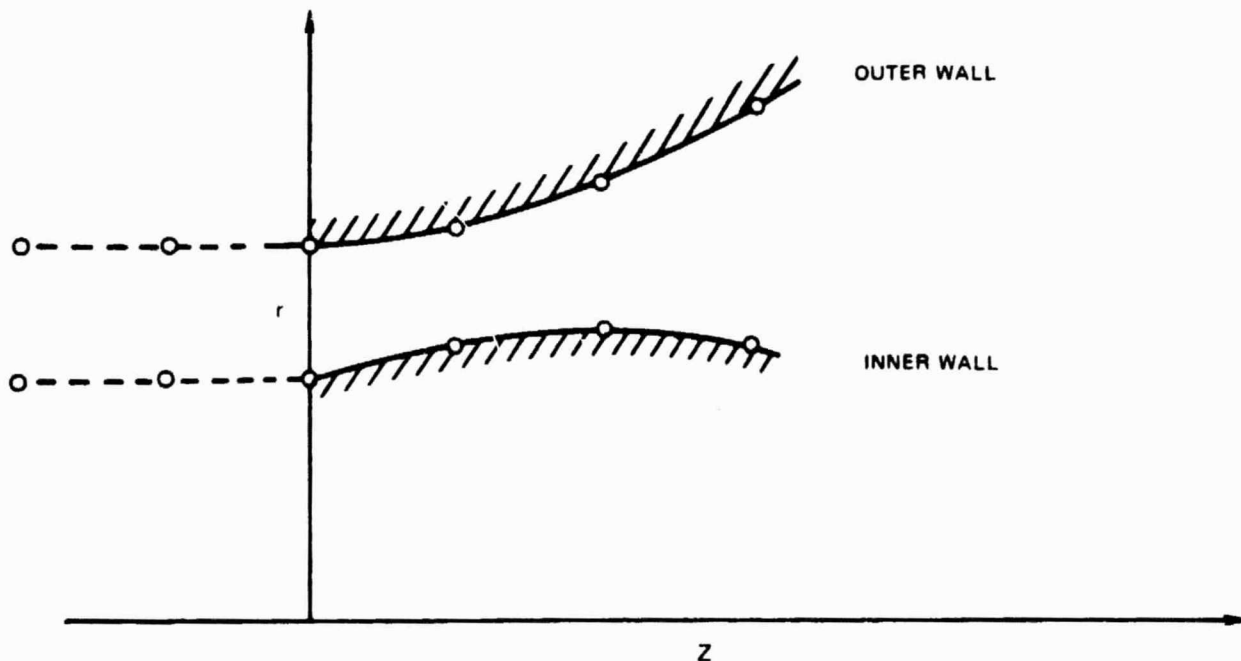
This error is detected in subroutine CASC. For blade and strut calculations use only $IØPT2=3$ with any ISHAPE, where

$$3 \leq \text{ISHAPE} \leq 6$$

Otherwise, the calculation will stop.

5) FOR BEST RESULTS ADD A STRAIGHT ANNULAR CHANNEL INLET

This error is detected in Subroutine C00R1. In the construction of the duct coordinates, it is assumed that the inlet has no curvature as shown in the figure below. This is not a fatal error because small inlet curvatures may be tolerated. For best results add a straight annular section to the inlet as shown by the dotted lines in the figure.



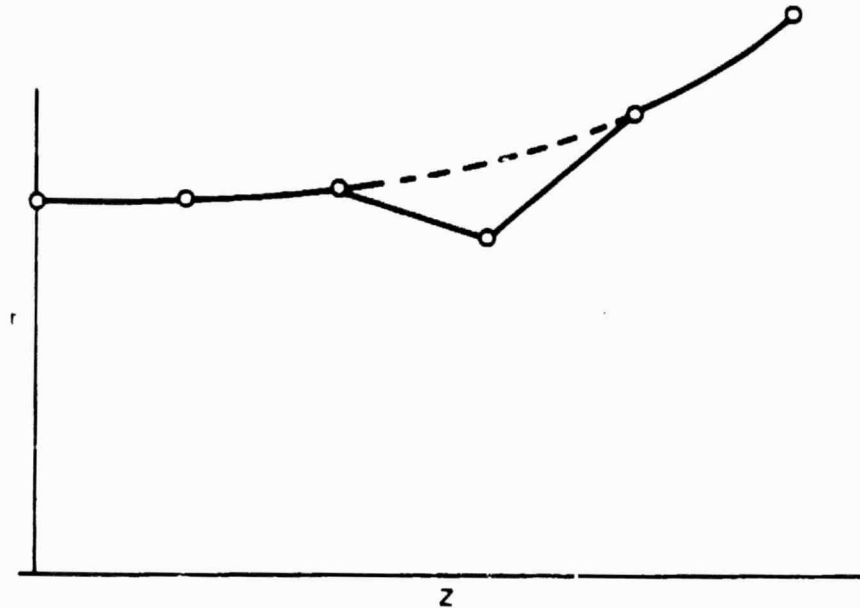
Addition of Straight Annular Channel Inlet

6) PROGRAM ASSUMES INLET FLOW HAS CURVATURE

This error is detected in Subroutine C00R1. Same as diagnostic 5.

7) WALL CURVATURE IS TOO LARGE AT STATION X.

This error is detected in Subroutine C00R1 usually if the duct has a discontinuous change in wall curvature such as shown in the figure below.



Discontinuous Change in Wall Curvature

8) Not Used

9) GREATER THAN 1. PERCENT NORMAL PRESSURE GRADIENT ERROR RECALCULATE STATIC PRESSURE

This error is detected in Subroutine ERPIN. This subroutine integrates the radial momentum equilibrium equation.

$$P_T - P_H = \gamma M^2 r^2 \int_0^1 \left[-\frac{\rho}{V} \frac{\partial V}{\partial n} U_s^2 + \frac{\rho}{R} \frac{\partial R}{\partial n} U_\phi^2 \right] \frac{dn}{XV}$$

and compares $(P_T - P_H)$ to that computed for the input inlet flow $(P_T - P_H)_1$. If the error given by

$$E = \left| 1 - \frac{P_T - P_H}{(P_T - P_H)_1} \right|$$

is greater than 0.01, the input initial static pressure distribution is replaced by the above pressure equation and the inlet flow is recalculated.

10) Not Used

11) MASS FLOW REQUIRED EXCEEDS MAXIMUM MASS FLOW POSSIBLE

This error is detected in Subroutine CKINPT. If it is determined that choked flow exists in the duct, this diagnostic will be printed; the weight flow must be reduced.

12) PRESSURE RISE EXCEEDS PERMISSIBLE PRESSURE RISE

This error is detected in Subroutine CKINPT and indicates that the deck cannot calculate properly the initial flow profiles. Check input for errors.

13) ITERATION OF BACK PRESSURE CALC. FAILS TO CONVERGE

This error is detected in Subroutine FINVIS.

In the calculation of strut forces, it has been assumed that the strut exit flow is subsonic and unseparated (i.e., $U_s > 0$). If these conditions are violated, no solution can be obtained. The calculation will stop.

14) BOUNDARY LAYER TOO THIN FOR MESH SPACING

This error is detected in Subroutine FLOWIN. The viscous flow calculation requires a finite initial boundary layer thickness. In addition, it requires enough mesh points to describe the inlet boundary layer velocity profile. The deck assumes arbitrarily that at least five mesh points are required. Thus, if this diagnostic occurs, increase the number of mesh points, KL, increase the mesh distortion parameter, DDS, or increase the assumed inlet boundary layer thickness. If DDS is input equal to zero, the program automatically sets the mesh distortion parameter to the appropriate value for turbulent flow.

15) TOTAL PRESSURE IS LESS THAN STATIC PRESSURE

This error is detected in Subroutine FLOWIN. A check is made on the input data for IOPT1 = 4 to make sure that $P_T > P$.

16) INPUT DATA NOT IN RADIAL EQUILIBRIUM CORRECTIONS APPLIED TO STATIC PRESSURE

This error is detected in Subroutine FLOWIN. A check is made of the input static pressure data for IOPT1 = 4. If the static pressure data are not in radial equilibrium, it is assumed that the static pressure data are in error and that the other inlet data are correct. Then the static pressure profile is computed from

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$$\frac{d\Pi}{d\eta} = 2 \frac{\gamma}{\gamma-1} \left[\frac{-1}{XV} \frac{\partial V}{\partial n} \cos^2 \alpha - \frac{1}{XR} \frac{\partial R}{\partial n} \sin^2 \alpha \right] \Pi \left(\left(\frac{\Pi_0}{\Pi} \right)^\gamma - 1 \right)^{\frac{1}{2}}$$

with the ID wall static pressure as a boundary condition.

17) INPUT DDS MUST BE SPECIFIED

This error is detected in Subroutine FNORM. At this time there is no algorithm to select automatically the mesh distortion parameter DDS for laminar flow.

18) BLADE DATA ERROR IN CKINPT ROUTINE

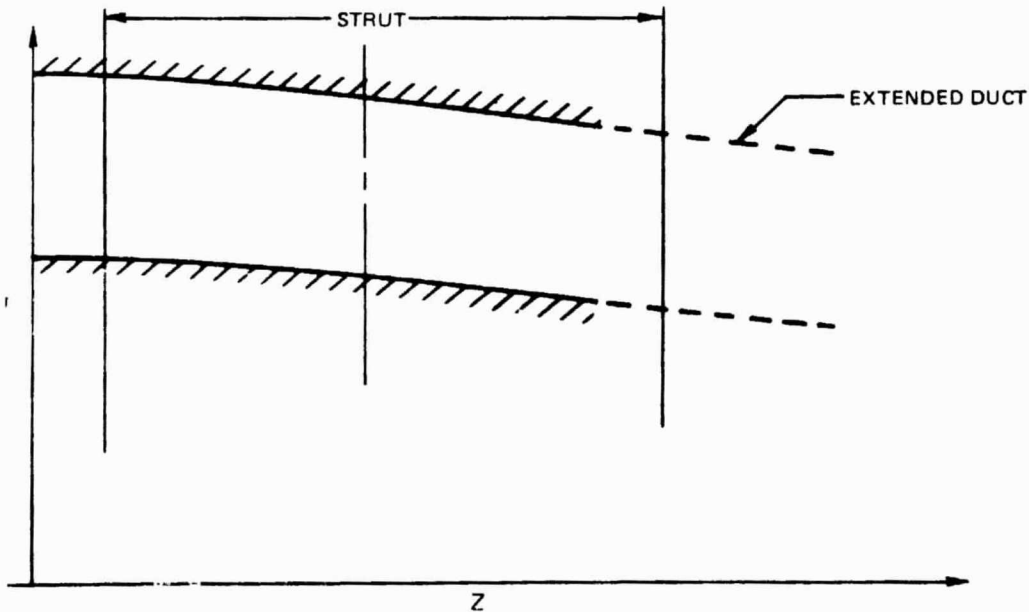
This error is detected in Subroutine CKINPT. Blade data have been input incorrectly and must be rearranged with Y increasing.

19) NO UNIQUE SOLUTION FROM MINVRT

This error is detected in Subroutine MINVRT. If the matrix used to solve for the turbulent flow solution is singular, no solution can be obtained. This situation may occur due to numerical truncation errors.

20) LEADING OR TRAILING EDGE INDEX OF STRUT OUT OF RANGE

This error is detected in Subroutine SLETE. In order to compute blade forces, the strut must be located entirely within the duct length. This problem may be eliminated by extending the duct as shown in the figure.



Extended Duct Section

21) SLOT INPUT NOT IN INCREASING ORDER

This error is detected in Subroutine SLØTA.

The slot input data must be arranged in order of increasing axial distance. Check input data. The calculation stops if this error is detected.

22) CHOKED FLOW IN SLOT NO.

This error is detected in Subroutine SLTFLØ. The slot weight flow is determined by the ratio of the stagnation pressure of the slot coolant fluid to the local wall static pressure. If this pressure ratio is too large the flow may be choked at the slot inlet. The calculation will stop.

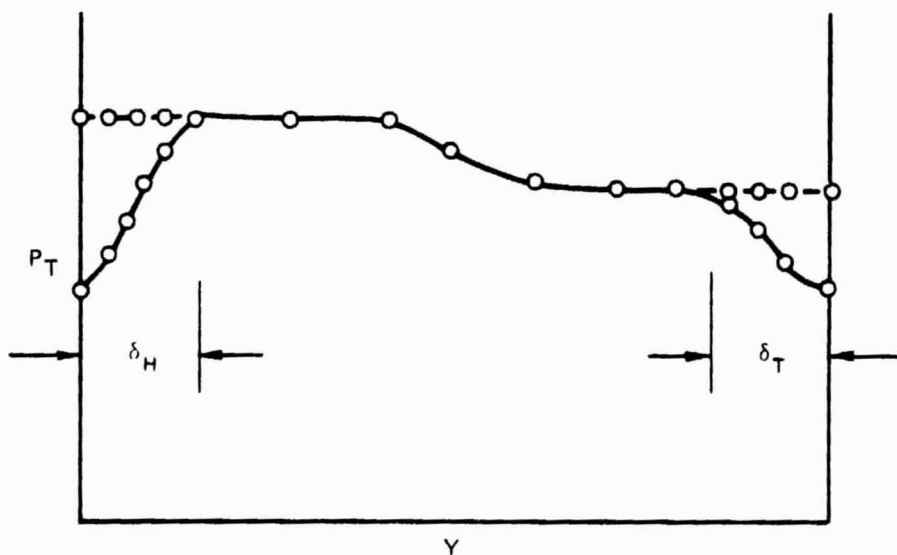
23) BOUNDARY LAYER OVERLAP OR TOO LARGE

This error is detected in Subroutine FLØWIN. For internal flow, the sum of the boundary layer thicknesses on the hub and tip walls must be less than the duct inlet height. Check input data.

24) SET TOTAL TEMPERATURE, PRESSURE, ANGLE TO VALUE AT EDGE OF BOUNDARY LAYER
- CORRECTIONS APPLIED

This error is detected in Subroutine FLØWIN. For IØPT1 = 4, the calculated boundary layer profiles are matched to input inlet flow profiles.

A good match requires that the stagnation pressure, P_T , be constant in the experimentally determined boundary layer region as shown in the figure (dashed line).



Constructing the Inlet Flow

25) TRUNCATION ERROR CANNOT BE REDUCED BY STEP SIZE

This error is detected in Subroutine SØLVI. If the step size parameter (KDS) is not specified, it is selected automatically by checking the truncation error at each step. When an instability occurs, the program attempts to reduce the truncation error by reducing the streamwise step size. If the truncation error cannot be reduced below a minimum value, the calculation stops.

26) NUMERICAL INSTABILITY

This error is detected in Subroutine FØRCE and Subroutine SØLVI and is an indication that the program has calculated negative temperatures or pressures. The calculation stops if this problem occurs.

27) RHOCX ITERATION DID NOT CONVERGE, ERR =

This error is detected in Subroutine FØRCE. In determining the blade force, an iteration scheme is used to determine the downstream static pressure. If this iteration fails to converge, this diagnostic is printed together with the maximum error found in the iteration. The calculation, however, is not terminated.

28) IOPT3 = 2 OPTION NOT IN USE

This error is detected in Subroutine FØRCE but this option has been deleted from the current version of the ADD code.

29) SOLUTION REQUIRES REVERSE FLOW, INCREASE WFLOW

This error is detected in Subroutine CKINPT. For flows with radial pressure gradients, there is a minimum weight flow below which reverse flow exists. This problem can be corrected by increasing the weight flow. The calculation will stop.

30) LOAD DOWNSTREAM FLOW DATA CARDS

This error is detected in subroutine CALINV and indicates that the downstream flow data cards, required by IOPT1 = 4 or 9, have not been entered. The calculation will stop.

31) SOLUTION FOR BLADE FORCE DOES NOT EXIST

This error is detected in subroutine FØRCE. The blade force cannot be calculated because no inviscid flow solution can be calculated. (Same as DIAGNØSTIC 29) The calculation will stop.

- 32) GRADIENT OF METRIC COEFFICIENT =
FOR BETTER RESULTS ADD STRAIGHT CHANNEL INLET

This error is detected in Subroutine C00R4. It is assumed that the inlet duct has no curvature. To avoid problems, add a straight annular section to the inlet. The calculation will continue.

- 33) INPUT TOO LARGE FOR COLE'S LAW
SET N < ____

This error is detected in subroutine FLOWIN.

Cole's friction law requires a certain relationship $H_{12} = H_{12} (R_e)$ such that there is an upper bound of $n < 10$. For a solution to exist,

$$A = \kappa \frac{Ue}{U^*} \left(1 - \frac{1}{H_{12}} \right) > 1.573$$

Setting

$$H_{\min} = 1 - \frac{1}{\frac{\kappa Ue}{U^*}}$$

Then

$$n < \frac{2}{H_{\min} - 1}$$

The calculation will stop.

- 34) WEIGHT FLOW ITERATION MAY NOT CONVERGE IN SUBROUTINE CKINPT CHECK INPUT DATA.

This error is detected in Subroutine CKINPT. The weight flow iteration that determines the static pressure may not converge if the free stream inviscid flow is highly distorted. An input flow which is more uniform in stagnation pressure is required. The calculation will stop.

- 35) WFLI AND I0PT11 OPTIONS INCOMPATIBLE

This error is detected in subroutine ALTMN. The weight flow cannot be specified for external flow. The calculation will stop.

- 36) I0PT1 = 1 OR I0PT1 = 2 OPTIONS NOT USED

This error is detected in Subroutine ALTMN. The options I0PT1 = 1 and I0PT1 = 2 have been deleted from the code.

- 37) CONFLICT OF OPTIONS, IOPT14<0 IMPLIES SEPARATION AND GLOBAL ITERATIONS.
AUTOMATIC STEP SIZE ALGORITHM CANNOT BE USED.

This error is detected in Subroutine SOLVI. When performing a global iteration (IOPT14>0), the same number of streamwise steps must be used for each iteration. Hence the automatic step size algorithm for the streamwise direction must not be used. The calculation will stop.

4.5 Debug Options for ADD Code

When set equal to unity, these options allow intermediate results calculated by the subroutine indicated to be printed as an aid in debugging a troublesome case. Note that these outputs are not converted to metric units and reference must be made to the source code for interpretation of printout.

| <u>OPTION</u> | <u>SUBROUTINE</u> | <u>OBJECTIVE OF SUBROUTINE</u> |
|---------------|-------------------|---|
| IDBG1 | TURB | Calculates two-layer turbulence model |
| IDBG2 | FCØRCT | Calculates shear stresses and heat fluxes at each station |
| IDBG3 | FLØWIN | Generates initial flow profiles |
| IDBG4 | SLTFLØ | Calculates slot inlet flows |
| IDBG5 | SØLVI | Calculates viscous flow solutions |
| IDBG6 | CØØR | Generates required geometric parameters |
| IDBG7 | FØRCE | Calculates forces generated by struts and blades |
| IDBG8 | MINVRT | Inverts a matrix |
| IDBG9 | SMØØTH | Smooths duct contour read via IØPT3 = 2 |
| IDBG10 | GDUCT | Calculates duct geometry |
| IDBG11 | SLTFLØ | Obtains additional information from SLTFLØ - see IDBG4 |
| IDBG12 | SØLVI | Obtains additional information from SØLVI - see IDBG5 |
| IDBG13 | CKINPT | Checks inlet flow input for errors |
| IDBG14 | SØLVI | Debugs the algorithm that automatically computes the maximum step size in the stream-wise direction while assuring computational stability. |
| IDBG15 | Not used. | |
| IDBG16 | Not used. | |
| IDBG17 | Not used. | |

4.6 Sample Input for ADD Code

Two sample inputs to the ADD code are presented on the following pages. These cases correspond to the two design studies described in Vol. I Section 7.0. The first sample is the input for the Swirl Tube Premixing Passage Case and the second sample is the input for the Series Staged Premixing Passage Case.

Swirl Tube Premixing Passage

The option card (line 2) indicates that the inlet flow conditions are to be calculated from input flow profile data (IØPT1=9). The duct geometry is to be determined using the straight wall annular diffuser option (IØPT3=3). Only the solution at every 5th station is to be printed (IØPT4=5) and the coordinates are to be read from a previously calculated data file (IØPT9=3). The mesh parameter card (line 3) indicates that the default mesh distortion parameter (DDS = 0.0) and step size (KDS = 0) algorithms are to be used. Two sets of 26 input data cards each describing the inlet and exit flow profiles, respectively, will be read. The duct geometry card (line 4) indicates that the overall duct length is 11.1 cm and that the inlet radius is 2.8956 cm. The inlet flow card (line 5) shows that the initial boundary layer displacement thickness is 0.029 cm and that a 1/7 power law profile is assumed for each wall. Lines 6 through 31 are the KLL=26 inlet flow profile data cards and lines 32 through 57 are the KLL-26 exit flow profile data cards which are identical to the inlet flow cards. The last card indicates that default values are used for the remaining input parameters except for the Prandtl number, heat capacities, and molecular viscosity.

Series Staged Premixing Passage

The option card (line 2) indicates that the inlet flow is to be calculated assuming a constant stagnation pressure and stagnation temperature in the core flow (IØPT1=3). The duct geometry is to be read from input data cards (IØPT3=2). On the mesh parameter card (line 3), the default mesh distortion parameter (DDS=0) has been selected but the streamwise step size parameter has been input KDS=2. From line 3, it is noted that the duct coordinates at JLPTS=50 equally spaced axial stations are to be read and that the least squares spline smoothing routine will be used (JLPTS ≠ JL). The length of the duct is 22.72 cm (line 4). Lines 5 through 11 contain 50 data points for the tip radii and lines 12 through 18 contain 50 data points for the hub radii. The inlet Mach number is 0.102 (line 19), the stagnation pressure is 11.06 atm, and the stagnation temperature is 745K.

5.0 OPERATION OF PTRAK CODE

5.1 Runstreams for PTRAK Code

Autoignition Model Not Used

It is assumed that:

1. The program will be executed in TPF\$;
2. The executable (absolute) element is PTRACK7;
3. The catalogued files, EIGHT and NINE, exist and have been written into by the ADD code (see ADD code input format);
4. A catalogued file exists for storing the fuel vaporization terms for use with the VAPDIF code (and is called SEVENTEEN in this example).

Then the following runstream is sufficient to execute the PTRAK code.

```
@ASG,AX EIGHT.,D/O/TRK/300000
@ASG,AX NINE., D/O/TRK/250000
@USE 8,EIGHT
@USE 9,NINE
@ASG,T 12,D/700000/TRK
@ASG,T 14,D/60000/TRK
@ASG,AX SEVENTEEN.,D/O/TRK/300000
@USE 17,SEVENTEEN
@ASG,T 18
@ASG,T 19
@XQT PTRACK7
(INPUT CARDS)
@FREE 8
```

@FREE 9

@FREE 12

@FREE 14

@FREE 17

@FREE 18

@FREE 19

Autoignition Model User'

It is assumed that:

1. The program will be executed in TPF\$;
2. The executable (absolute) element is PTRACK7;
3. The catalogued files, EIGHT and NINE, exist and have been written into by the ADD code (see ADD code input format);
4. A catalogued file exists for storing the fuel vaporization terms for use with the VAPDIF code (and is called SEVENTEEN in this example).
5. A catalogued file exists for storing the critical species source terms for use with the VAPDIF code (and is called TWENTYSEVEN in this example);
6. A catalogued file exists for storing the temperature depression source terms for use with the VAPDIF code (and is called TWENTYEIGHT in this example).

Then the following runstream is sufficient to execute the PTRAK code when using the autoignition model.

@ASG,AX EIGHT.,D/O/TRK/300000

@ASG,AX NINE., D/O/TRK/250000

@USE 8,EIGHT

@USE 9,NINE

@ASG, 12,D/700000/TRK

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@ASG,T 14,D/60000/TRK

@ASG,AX SEVENTEEN.,D/O/TRK/300000

@USE 17,SEVENTEEN

@ASG,T 18

@ASG,T 19

@ASG,AX TWENTYSEVEN.,D/O/TRK/300000

@USE 27,TWENTYSEVEN

@ASG,AX TWENTYEIGHT.,D/O/TRK/300000

@USE 28,TWENTYEIGHT

@XQT PTRACK7

(INPUT CARDS)

@FREE 8

@FREE 9

@FREE 12

@FREE 14

@FREE 17

@FREE 18

@FREE 19

@FREE 27

@FREE 28

5.2 Input Format for PTRAK Code

The input to the PTRAK code is described on the input data coding forms which follow. These coding forms are arranged with one form per input data card. Each form contains the names of the input variables, the format, and a description of the data. In general, the input data is read as follows:

- Card 1 Title Card
- Card 2 Option Card
- Card 3 Fuel Class Description Card
- Card 4 Injector Description (ILØC) Cards
- Card 5 Initial Velocity (ILØC) Cards
- Card 6 Fuel Flow Rate Card
- Card 7 Fuel Thermodynamic Constants Card
- Card 8 Fuel Thermodynamic Functions (6) Cards
- Card 9 Air Thermodynamic Constants Card
- Card 10 Air Thermodynamic Functions (3) Cards
- Card 11 Mesh Description Card
- Card 12 Distillation Curve (IDSTL+1) Cards
- Card 13 Collision Data Card
- Card 14 Cox Chart Data Cards (ICØX1+1) Cards
- Card 15 Autoignition Model Constants (3) Cards

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PTRAK CODE INPUT

Card 1 TITLE CARD FORMAT (12A6)

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---------------------|----|----|----|----|----|----|----|----|----|----------------------|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 0 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 | 39 | 40 | 41 | 42 | 43 | 44 | 45 | 46 | 47 | 48 | 49 | 50 | 51 | 52 | 53 | 54 | 55 | 56 | 57 | 58 | 59 | 60 | 61 | 62 | 63 | 64 | 65 | 66 | 67 | 68 | 69 | 70 | 71 | 72 | 73 | 74 | 75 | 76 | 77 | 78 | 79 | 80 |
| | | | | | | | | | | FIRST LINE OF TITLE | | | | | | | | | | SECOND LINE OF TITLE | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

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IØPT5 Last Axial Station for Performing Trajectory Calculations.
If Omitted, Program will Use "JL" From ADD Run

IØPT6 (Friction Drag Option)
= 0 Use Droplet Drag Coefficient Correlations
= 1 Set Drag Coefficients to Zero

IØPT7 (VAPDIF Storage Option)
= 0 No Information Is Stored on Unit 17
= 1 Store Vapor Source Terms on Unit 17
= 2 Store vapor, critical species and temperature depression source terms
(on units 17, 27, and 28, respectively) for autoignition Model I (see
Volume I, Section 8.0)
= 3 Same as IØPT7 = 2 but for Model II

Note: Debug options are described in Section 5.5

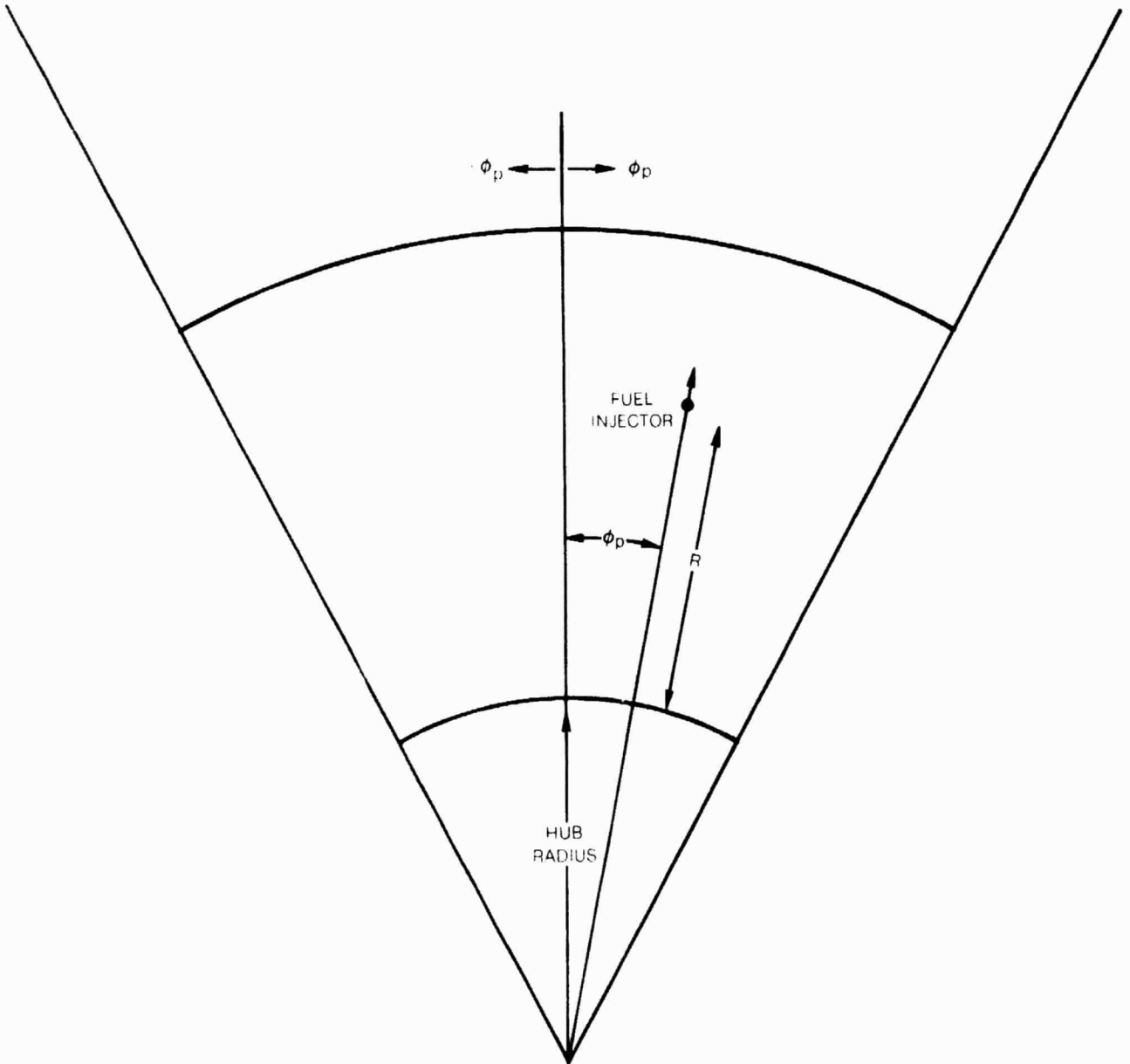
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FIG. 5.1

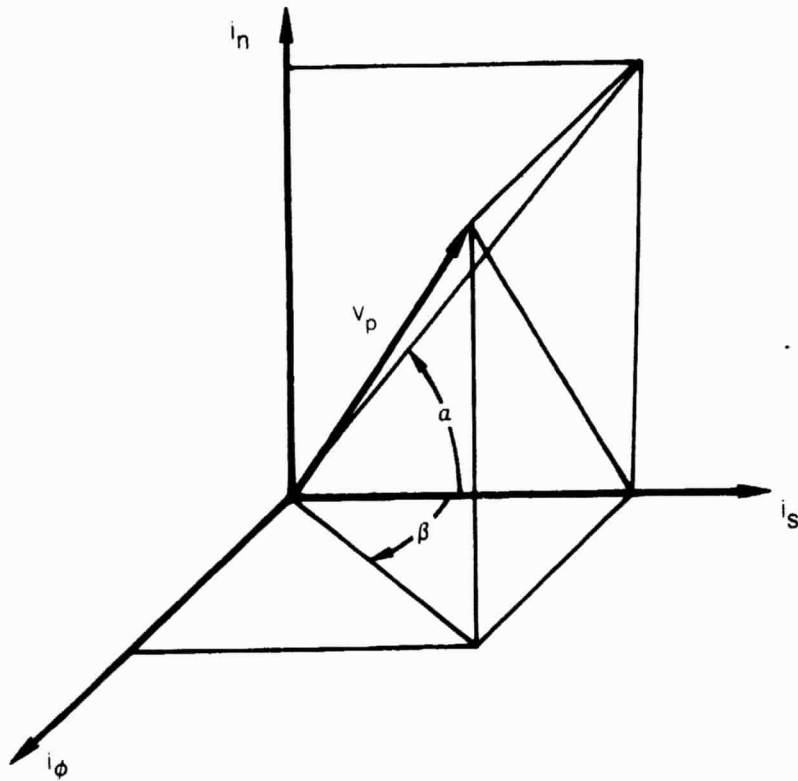
FUEL INJECTOR DESCRIPTION

(CARD NO. 4)



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INPUT DROPLET VELOCITY VECTORS



$$\text{TAN } \alpha = v_n / v_s$$

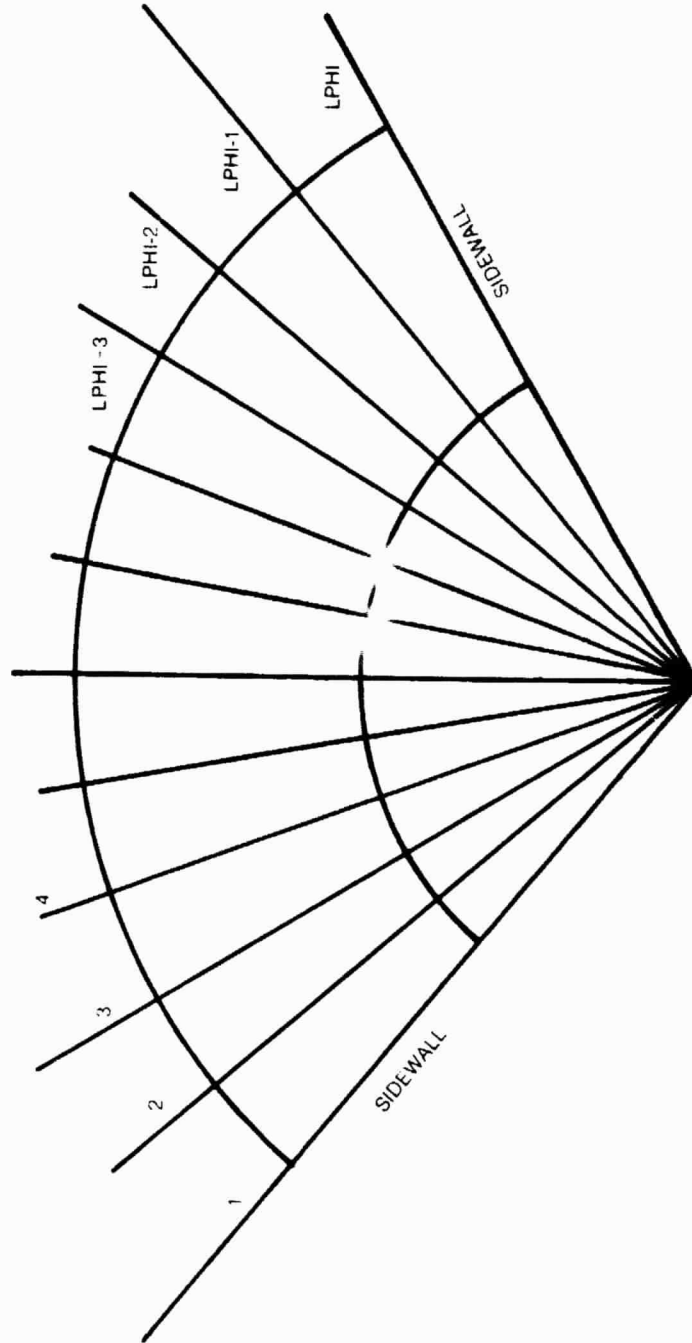
$$\text{TAN } \beta = v_\phi / v_s$$

$$v_{\text{MEAN}} = |\vec{v}_p|$$

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DEFINITION OF LATERAL EXTENT OF DUCT FOR PTRAK

(CARD NO 11)



Cox Chart for the Simulation of a Pure Substance

The Cox Chart for simulating a pure substance consists of (a) a set of arbitrary "carbon" numbers, COX(1); (b) a set of arbitrary temperatures for a vapor pressure of P1CH, COX(2); and (c) a set of temperatures all of which are equal to the temperature that produces a vapor pressure of P2CH, COX(3). At any point in the calculation, the program will obtain the distillation temperature for the instantaneous value of percentage of fuel evaporated (this temperature for a pure substance is the normal boiling point), calculate an obviously meaningless "carbon" number, and then find the temperature that produces a vapor pressure equal to P2CH. These parameters are sufficient to calculate the vapor pressure at the instantaneous value of droplet temperature (see Volume I, Section 4.5). A Cox chart for the normal paraffin series is given in Table 5.1.

TABLE 5.1

COX CHART FOR NORMAL PARAFFIN SERIES

P1CH = 1 atm
P2CH = 6.8 atm

| <u>Carbon No.</u> | <u>T@P1CH (deg K)</u> | <u>T@P2CH (deg K)</u> |
|-------------------|-----------------------|-----------------------|
| 2 | 175 | 225 |
| 3 | 230 | 285 |
| 4 | 270 | 335 |
| 5 | 310 | 380 |
| 6 | 345 | 420 |
| 7 | 370 | 455 |
| 8 | 405 | 485 |
| 9 | 430 | 515 |
| 10 | 455 | 540 |
| 11 | 475 | 570 |
| 12 | 490 | 590 |
| 13 | 510 | 605 |
| 14 | 530 | 625 |
| 15 | 545 | 640 |
| 16 | 560 | 660 |
| 17 | 580 | 675 |
| 18 | 588 | 690 |
| 19 | 605 | 700 |
| 20 | 620 | 715 |
| 23 | 640 | 740 |

5.3 Output Description for PTRAK Code

The output on each page from the PTRAK code is largely self-explanatory. A general description of the output by page is given below.

Title Page

This page presents a list of modifications, dates, and references to all changes to the PTRAK code.

Option Page

This page lists all options used in the PTRAK calculation and the number of classes in each category.

Fuel Injector Page

This page lists the location and initial conditions for all fuel injectors. The total fuel flow rate is also printed.

Fuel Thermodynamic Properties Page

This page presents the thermodynamic data and transport properties for both the fuel liquid and vapor phases.

Air Thermodynamic Properties Page

This page presents both the thermodynamic data and transport properties for the air and the mesh parameters.

Multicomponent Fuel Properties Page

This page lists the data for the distillation curve and Cox chart.

Autoignition Model Constants Page

This page lists all constants used in the autoignition model.

Initial Conditions by Class Page

This page describes the initial conditions, including number density, for all droplet classes.

Duct Geometry Page

This page presents the coordinates of the duct contour.

Solution Pages

These pages present all of the dependent variables by class, and the overall Sauter mean diameter, number of droplets, and fuel flow rate at each axial station.

Summary Page

The summary page presents the global properties of the fuel spray and includes the Sauter mean diameter, liquid fuel flow rate, percentage of fuel evaporated, and fuel-air ratio as a function of axial distance.

5.4 Diagnostics for PTRAK Code

Numerous checks are made during the course of the calculation. If a minor error occurs, a DIAGNOSTIC message is printed and the calculation continues. If a fatal error occurs, a DIAGNOSTIC is printed and the calculation is stopped. A description of these errors is given in this section. The DIAGNOSTIC message is always of the form

****DIAGNOSTIC NO. XX FOR PTRAK CODE****

where xx refers to one of the errors listed below.

1. FAILURE TO INTERPOLATE IN FINTP

This error occurs when the PTRAK code cannot find the location where a particle track crosses a grid point. The axial step-size should be reduced by increasing KDS. This error causes the calculation to terminate.

5.5 Debug Options for PTRAK Code

When set equal to unity, these options allow intermediate results calculated by the subroutine indicated to be printed as an aid in debugging a troublesome case. These outputs are not converted to metric units and reference must be made to the source code for interpretation of the printout.

| <u>OPTION</u> | <u>SUBROUTINE</u> |
|---------------|-------------------|
| IDBG1 | PTRAK |
| IDBG2 | BØUNCE |
| IDBG3 | CØLLSM, COLLDB |

5.6 Sample Input for PTRAK Code

This sample of input to the PTRAK code is based on the Series Staged Premixing Passage case described in Volume I, Section 7. The option card (line 2) indicates that the duct is an annular passage with periodic boundary conditions ($I\theta PT3=4$). Thus the inner and outer boundaries are to be treated as solid walls and the two remaining boundaries represent the lateral extent of the annular segment being considered. While the air flow in this case is not swirling, droplets injected normal to the flow direction but in the angular direction may exit from this segment to an adjacent segment. If droplets do exit through one of the "sidewalls", then a source of droplets identical in all respects to this sink of droplets must enter this segment through the opposite sidewall. Only the behavior of the spray in a 1/60th segment of the annular duct is to be calculated ($LPHI = 31$ and $DPHI = 0.2$ from line 24). From line 5, the fuel class description card, there are four injectors ($IL\theta C = 4$) and only one class is to be formed at each injection location using the binominal distribution function for each property. Thus, the total number of droplet classes is four. These four injectors, described on lines 4 through 7, are located 7.48 cm from the inlet. Lines 8 through 11 describe the initial velocity components and droplet size for each injector. The fuel flow rate is .01146 kg/sec (line 12). The thermodynamic and transport data for the fuel and air are presented on lines 13 through 23. The distillation curve appears on lines 25 through 31 and the Cox chart is listed on lines 33 through 53. All droplets which strike a solid wall will rebound elastically (line 32, $C1 = 1.0$).

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TRACK FOR PARAMETRIC 2 - PENETRATING UNITS, 1/60TH SEGMENT

| Line | Code | Value | Code | Value | Code | Value | Code | Value |
|------|------|--------|------|-------|------|-------|------|-------|
| 1 | 4 | 1.1958 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 2 | 4 | 1.6252 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 3 | 4 | 1.9154 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 4 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 5 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 6 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 7 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 8 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 9 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 10 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 11 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 12 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 13 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 14 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 15 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 16 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 17 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 18 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 19 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 20 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 21 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 22 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 23 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 24 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 25 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 26 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 27 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 28 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 29 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 30 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 31 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 32 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 33 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 34 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 35 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 36 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 37 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 38 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 39 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 40 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 41 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 42 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 43 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 44 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 45 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 46 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 47 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 48 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 49 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 50 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 51 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |
| 52 | 4 | 0.0 | 0 | 0.0 | 0 | 0.0 | 0 | 0.0 |

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6.0 OPERATION OF VAPDIF CODE

6.1 Runstreams for VAPDIF Code

Calculation of Fuel Vapor Mass Fraction Distribution

It is assumed that:

1. The program will be executed in TPF\$;
2. The executable (absolute) element is DIFFUSEMAP;
3. The catalogued files, EIGHT and NINE, exist and have been written into by the ADD code;
4. The catalogued file, SEVENTEEN, exists and has been written into by the PTRAK code;
5. The catalogued file, FUELSØL, exists and will be written into by the VAPDIF code. It is used to permit the VAPDIF code to restart a case subsequent to the initial run. If no restart capability is desired, this file may be a temporary file. The file FUELSØL contains the solution of the diffusion equation at each mesh point for the fuel vapor mass fraction.

Then the following runstream is sufficient to execute the VAPDIF code.

```
@ASG,AX EIGHT,D/O/TRK/300000

@ASG,AX NINE,D/O/TRK/250000

@USE 8,EIGHT

@USE 9,NINE

@ASG,T 10,D/O/TRK/2250000

@ASG,AX FUELSØL,D/O/TRK/250000

@USE 11,FUELSØL

@ASG,T 12/D/O/TRK/750000

@ASG,T 13,D/O/TRK/2250000

@ASG,AX SEVENTEEN.,D/O/TRK/300000

@USE 17,SEVENTEEN
```

@XQT DIFFUSEMAP

(INPUT CARDS)

@FREE 8

@FREE 9

@FREE 10

@FREE 11

@FREE 12

@FREE 13

@FREE 17

Calculation of Critical Species Concentration Distribution

The mass fraction of critical species (ethene when using autoignition Model I) or of the relative mass fraction of the unknown critical species (using autoignition Model II) can be calculated using the following runstream once the fuel vapor mass fraction distribution is known.

It is assumed that:

1. The program will be executed in TPF\$;
2. The executable (absolute) element is DIFFUSEMAP;
3. The catalogued files, EIGHT and NINE, exist and have been written into by the ADD code;
4. The catalogued files, SEVENTEEN, TWENTYSEVEN and TWENTYEIGHT have been written into by the PTRAK code;
5. The catalogued file, ELEVEN, exists and will be written into by the VAPDIF code. It is used to permit the VAPDIF code to restart a case subsequent to the initial run. If no restart capability is desired, this file may be a temporary file. The file ELEVEN contains the solution to the diffusion equation at each mesh point for the concentration of critical species.
6. The catalogued file, FUELSØL, exists and contains the fuel vapor mass fraction distribution determined previously by the VAPDIF code.

Then the following runstream is sufficient to execute the VAPDIF code when using the autoignition model.

@ASG,AX EIGHT,D/O/TRK/300000

@ASG,AX NINE,D/O/TRK/250000

@USE 8,EIGHT

@USE 9,NINE

@ASG,T 10,D/O/TRK/2250000

@ASG,AX ELEVEN,D/O/TRK/250000

@USE 11,ELEVEN

@ASG,T 12/D/O/TRK/750000

@ASG,T 13,D/O/TRK/2250000

@ASG,AX SEVENTEEN.,D/O/TRK/300000

@USE 17,SEVENTEEN

@ASG,AX FUELSØL.,D/O/TRK/250000

@USE 19,FUELSØL

@ASG,AX TWENTYSEVEN.,D/O/TRK/300000

@USE 27,TWENTYSEVEN

@ASG,AX TWENTYEIGHT.,D/O/TRK/300000

@USE 28,TWENTYEIGHT

@XQT.. DIFFUSEMAP

(INPUT CARDS)

@FREE 8

@FREE 9

@FREE 10

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@FREE 11

@FREE 12

@FREE 13

@FREE 17

@FREE 19

@FREE 27

@FREE 28

6.2 Input Format for VAPDIF Code

The input to the VAPDIF code is described on the input data coding forms which follow. These coding forms are arranged with one form per input data card. In general the input data is read as follows:

- | | |
|--------|--|
| Card 1 | Title Card |
| Card 2 | Option Card |
| Card 3 | Print Option Card |
| Card 4 | Miscellaneous Data Card |
| Card 5 | Autoignition Model Constants (4) Cards |

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VAPDIF CODE INPUT

Card 1 TITLE CARD FØRMAT (12A6)

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-------|---|---|---|---|---|---|---|---|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 | 39 | 40 | 41 | 42 | 43 | 44 | 45 | 46 | 47 | 48 | 49 | 50 | 51 | 52 | 53 | 54 | 55 | 56 | 57 | 58 | 59 | 60 | 61 | 62 | 63 | 64 | 65 | 66 | 67 | 68 | 69 | 70 | 71 | 72 | 73 | 74 | 75 | 76 | 77 | 78 | 79 | 80 |
| TITLE | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

WR Relaxation parameter. If omitted, the value is obtained from an equation due to Garabedian:

$$WR = \frac{2}{1 + \lambda \bar{h}/A^{1/2}}$$

where

$$\bar{h} = \left(\left(\frac{Y_{2L}}{JL-1} \right)^2 + \left(\frac{Y_{3L}}{KL-1} \right)^2 \right)^{1/2}$$

$$A^{1/2} = (Y_{2L} * Y_{3L})^{1/2}$$

$$\lambda = 2.53878$$

A value of WR = 1.0 is recommended.

CZERØ Initial, uniform level of fuel vapor mass fraction in entrance plane.

6.3 Output Description for VAPDIF Code

The output on each page from the VAPDIF code is largely self-explanatory. A general description of the output by page is given below.

Input Page

The input page presents all of the input data including: options, computational grid size controls, iteration parameters, and the axial coordinates of the corner point ($J = 1$, $K = 1$). In addition the reference conditions for the ADD code viscous flow field are printed.

Source Term Pages

If $IPRNT4=1$, the source terms on the crossplane grid are printed. These terms are arranged by (K row), (J column) where K is the index for the tangential (azimuthal) coordinate and J is the index for the normal (radial) coordinate.

Solution Page

If $IPRNT1 = 0$, the mass fractions on the crossplane grid are printed.

Coordinate Grid Page

For $IPRNT2$ or $IPRNT3 \neq 0$, the coordinates on the crossplane grid are printed.

Iteration Page

If $IDB1 = 1$, the iteration history of the calculation is printed. This print-out includes the iteration number, residual, maximum concentration, and mass flow weighted average concentration for each residual.

Flow Summary Page

This page presents values of vapor flow rate and vapor fuel to air ratio as a function of axial location determined by integrating the vapor concentration over the crossplane grid at each axial station. The last column, labeled CTIL, is the overall vapor fuel to air ratio as determined by the PTRAK code and serves as a check of the accuracy of the VAPDIF calculation.

6.4 Diagnostics for VAPDIF

At the present time no diagnostics exist for the VAPDIF code.

6.5 Debug Options for VAPDIF Code

If the options IDB1, IDB2, IDB3 are set equal to unity, intermediate results are printed for each iteration.

| <u>Option</u> | <u>Data Printed</u> |
|---------------|--|
| IDB1 | Print maximum iteration residuals |
| IDB2 | Not used |
| IDB3 | Print coefficients of linearized equations |

The solution for each iteration at the point (J1DBG, K1DBG) on the calculation plane (crossplane grid) may also be printed. These terms are arranged by (K row), (J column) where K is the index for the tangential (azimuthal) coordinate and J is the index for the normal (radial) coordinate. Solutions for the points (J2DBG, K2DBG), (J3DBG, K3DBG), and (J4DBG, K4DBG) may also be displayed.

It is recommended that IDB1 be set equal to unity.

6.6 Sample Input for VAPDIF Code

The sample of input to the VAPDIF code is based on the Swirl Tube Premixing Passage case described in Volume I, Section 7. Since almost all input data required to run the code is stored in data files generated by the ADD and PTRAK codes, little input is required by the VAPDIF code. On card 2 (line 2), it is noted that the number of iterations is limited to $I\text{OPT}1=5$. The initial flowfield station is located at the first ADD code coordinate station ($I\text{ADD}=1$), the first calculation station after the initial plane is $I\text{BEGIN}=2$, and the calculation will terminate at station $I\text{END} = 5$. The print option card (line 3) indicates that both the concentrations and fuel source distributions will be printed at each station. The last card (line 4) shows that the Schmidt number is unity.

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VAPOR DIFFUSION CASE FOR PARAMETRIC CASE 1

5 1 2 5
000100
1.0

1
2
3
4

7.0 GLOBAL STRUCTURE

7.1 Interaction of ADD, PTRAK, VAPDIF Codes

The Global Structure Flow Chart which describes the interactions of the ADD, PTRAK, and VAPDIF codes is shown on Fig. 7.1. The three codes are executed independently in the sequential order shown and output stored on data files. The data files (Units 8, 9, 11, 17, 19, 27, 28) are the only interfaces between the codes.

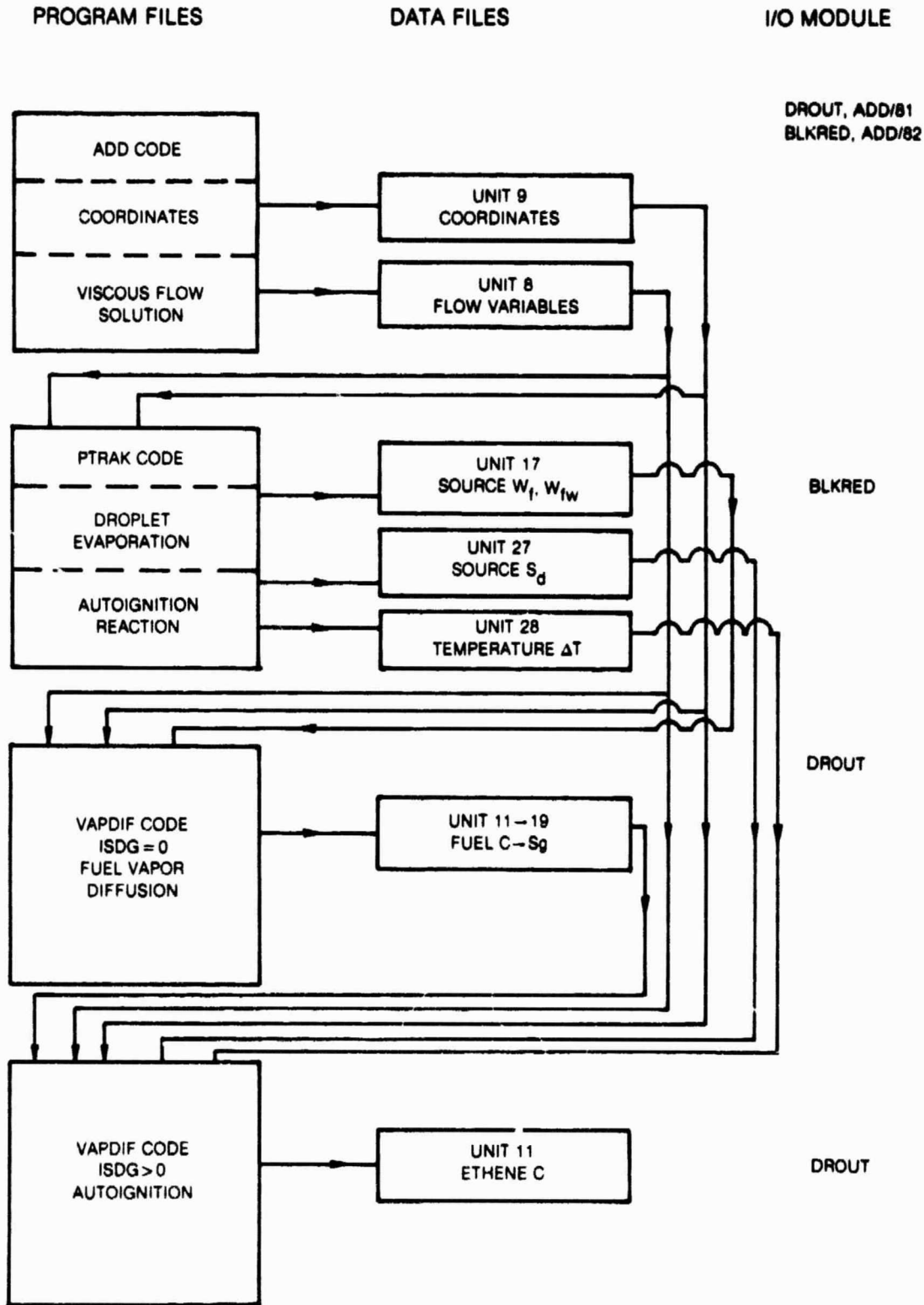
The ADD code calculates the computational coordinates (S,N) and physical cylindrical coordinates (r,z) and stores this data on Unit 9. This coordinate data is required by both the PTRAK and VAPDIF codes. The ADD code also calculates the viscous flow solution and stores the flow variables ($P, T, \rho, \vec{V}, \mu_E$) on Unit 8. These flow variables are required by both the PTRAK and VAPDIF. Certain control parameters, such as the number of streamlines KL and number of streamwise stations JL, which are required by the PTRAK and VAPDIF codes are also stored on Units 8 and 9 and are not required inputs to these codes. This procedure reduces conflicts or ambiguities when executing the three codes.

The PTRAK code calculates the droplet trajectories and degree of evaporation from the initial droplet conditions and known flow field. This solution is used to calculate the source terms \dot{W}_f and \dot{W}_{fw} which are stored on Unit 17 for use by the VAPDIF code. The PTRAK code also calculates preignition reactions and stores a source term S_d on Unit 27. As the droplets evaporate, they cool the surrounding air. This temperature drop ΔT is stored on Unit 28.

The VAPDIF code can be executed in two modes. The first execution, with ISDG=0, calculates the three dimensional fuel concentration throughout the flow field using the fuel source distribution calculated from the PTRAK code. This solution is written on Unit 11. On the second execution, ISDG=1 or 2, VAPDIF calculates the concentration of critical species. The fuel concentration which was previously written on Unit 11 is read on Unit 19 and used to calculate the source term due to chemical reaction in the gas phase. The critical species concentration is then stored on Unit 11.

It is noted that all control parameters are calculated and stored by the first code and are not required input to succeeding codes. This arrangement of codes produces considerable flexibility in that any data which is calculated and permanently stored on data files need not be repeated. As an example: for any given premixing duct and airflow conditions, several different droplet ejectors may be examined using the PTRAK code without repeating the ADD code calculation.

GLOBAL STRUCTURE FLOW CHART



7.2 Input/Output Data Files

The output data files for the ADD; PTRAK, and VAPDIF codes are described on Tables 7.1, 7.2, 7.3 respectively. These tables show the Unit number, the names of the arrays stored on the file, the block (record) length in words, the number of blocks (records), and the subroutine generating the files. All unit numbers are set by parameters statements (in brackets). All arrays are single precision except AFF generated by the ADD code.

In the operation of the ADD code, only files assigned to Units 8, 9, 11, and 22 are required. The other files are only used for special options in the ADD code which would not generally be used for a LPP duct calculation. Note also that only output files are shown under the computer code name. Input files for the PTRAK code are described on Table 7.1, and input files for the VAPDIF are described on Tables 7.1 and 7.2. The actual file assignments and runstreams for each code are described in Sections 4.1, 5.1, and 6.1.

These data files are read/written by general I/O routines DRØUT in the ADD/81 and VAPDIF codes or by BLKRED in the ADD/82 (Ref. 4) and PTRAK. These subroutines use the UNIVAC Library I/O routine NTRAN. Both DRØUT and BLKRED are easily converted to ANSI standard FORTRAN DEFINE FILE.

Table 7.1

Table of File Assignments ADD Code

| <u>UNIT NO.</u> | <u>ARRAY NAME</u> | <u>BLOCK LENGTH (WDS)</u> | <u>NO. BLOCKS</u> | <u>SUBROUTINE WRITING BLOCK</u> |
|---------------------|--|-------------------------------|-----------------------|-------------------------------------|
| 8 (NDRUM) | F(NEQ,3,IST) FPARM(15) | 3015 | JL-2 | SØLVI |
| 9(JDRUM) | JSTEP Q(19,IST) RHS(10) RMS(10) RTS(10) DSTEP QPARM(9) | 1941 | JL | CØØRST |
| 10(CDRUM) | FF(17,2,IST) | 3400 | 1 | FØRCE |
| 11(LDRUM) | AFF(LNGTO)** | 6000 | 5 | SØLVI |
| 12(LFØRC) | FØRC | 780 | 1 | FØRCE |
| 19(KPØIS) | JSTEP Q(19,IST) RHS(10) RMS(10) RTS(10) DSTEP QPARM(9) | 1941 | JL | CØØRST |
| 22(MDRUM) | FIV(NEQ,3,IST) FIPARM(15) | 3015 | JL-2 | CALINV |
| 23(NFDRM) | F(IST4) | 104 | JL+NST-2 | PØISCF |
| 24(NPDRM) | P(IST) | 100 | JL+NST-2 | PØIS |
| 25(NGDRM) | BLK(NGIST) | 400 | JL+NST-2 | PØISCF |

**Double precision variables

1S = 100

NST = 25

IST = 100

Table 7.2

Table of File Assignments PTRAK Code

| <u>UNIT NO.</u> | <u>ARRAY NAME</u> | <u>BLOCK LENGTH (WDS)</u> | <u>NO. BLOCKS</u> | <u>SUBROUTINE WRITING BLOCK</u> |
|---------------------|---|-------------------------------|-----------------------|-------------------------------------|
| 12(KTDRUM) | PART(200,13) | 2600 | JL | SMTER |
| 17(MDRUM) | AMASS(IST,50) RDUM(IST,4) APARM(10) | 5410 | JL | DATAM |
| 18(NBØUN) | RPART(IST,2) PHPART(IST,2) | 400 | JL | SMTER |
| 19(ISDRU) | SARRAY(8) | 8 | JL | SMTER |
| 27(MDRUK1) | AMASS(IST,50) RDUM(IST,4) APARM(10) | 5410 | JL | DATAM |
| 28(MDRUM2) | AMASS(IST,50) RDUM(IST,4) APARM(10) | 5410 | JL | DATAM |

JL ≤ IS = 100

KL ≤ IST = 100

Table 7.3

Table of File Assignments VAPDIF

| <u>UNIT NO.</u> | <u>ARRAY NAME</u> | <u>BLOCK LENGTH (WDS)</u> | <u>NO. BLOCKS</u> | <u>SUBROUTINE WRITING BLOCK</u> |
|---------------------|-----------------------|-------------------------------|-----------------------|-------------------------------------|
| 10(IYDRM) | Y(3,3,IST,10) | 45,000 | JL | ADDCØR |
| 11(IFDEM) | FG(IST,10) | 5,000 | JL | SØLVE |
| 12(IXDRM) | X(3,IST,10) | 15,000 | JL | ADDCØR |
| 13(ITCØR) | TCØR(3,3,IST,10) | 45,000 | JL | ADDCØR |

8.0 DETAIL DESCRIPTION OF PTRAK CODE

8.1 Main Program/Flow Chart

The flow chart for the main program PTRAK is shown on Fig. 8.1. It consists of three major tasks: 1) Read input data and set up initial conditions for the droplet (subroutines INPUT, INTIAL, ØUTPUT); 2) Calculate the droplet trajectory, evaporation rate, and production of critical species (subroutines TRACK, SUMRY); and 3) Calculate the source terms for use by the VAPDIF (subroutine DATAM).

In task 1, INPUT reads the input data according to the input format described in Section 4.2. INIT determines the initial droplet conditions (location, temperature, velocity, mass) which define the droplet classes by specifying number density distribution described in Section 4.7. ØUTPUT prints the input data and initial conditions.

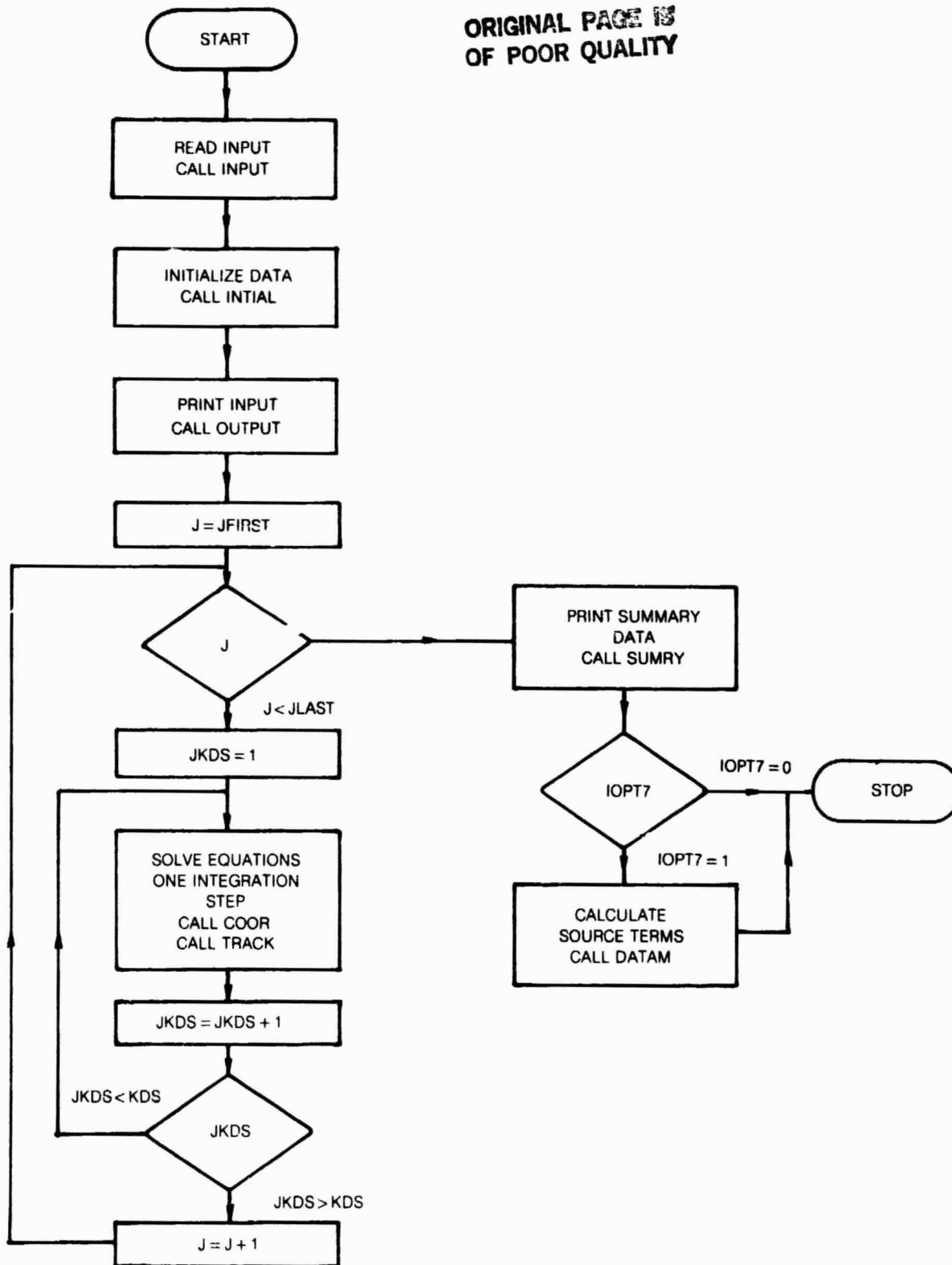
The integration of the droplet equations for one step is accomplished by subroutine TRACK using a fine coordinate grid interpolated from the course coordinate grid calculated by CØØR. The outer DØ loop indexes the course grid where the J index corresponds to the Jth streamwise coordinate (block) stored on file 9. The inner DØ loop indexes the fine grid in KDS interpolated steps using the index JKDS. The integration takes place from JFIRST to JLAST in KDS*(JLAST-JFIRST) steps. At the present time there is no algorithm for varying the step size KDS. As the integration proceeds, the solution at each Jth station for the droplet dependent variables is stored on file 12 and a summary of this data is stored on file 19. When the integration is complete, a summary of the solution is printed by SUMRY.

The execution of the third major task depends on the input option IØPT7. When IØPT7>0, subroutine DATAM searches through the solution files (8,9,12) calculates the source terms for the production of fuel, the source terms for the production of critical species, and the drop in air temperature due to droplet evaporation. These results are stored for each mesh point on the course grid corresponding to the coordinate grid stored on file 9.

FIG. 8.1

FLOW CHART FOR MAIN PROGRAM PTRAK

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OF POOR QUALITY



8.2 Description of Modules by Major Task

A complete list and brief description of all the subroutines is given in Section 8.3. The flow chart for the main program PTRAK is shown on Fig. 8.1 and an overall description is given in Section 8.1. The description of the module functions will follow this flow chart. Only major computational tasks will be described. Minor tasks and Input/Output are self explanatory and will not be described.

Following through the flow chart Fig. 8.1, the first major task is performed by subroutine INTIAL which stores the crosssection boundary at the initial station on unit NB \emptyset UND, reads the flow field variables at the initial station from unit NDRUM, and calculates the initial droplet conditions by calling subroutine FN \emptyset Z. FN \emptyset Z specifies the initial conditions (Eqs. 4.7.1), and specifies the number density in phase space defined by (Eq. 4.7.2). Generally the binomial distribution (Eq. 4.7.3) calculated by FBIN is used. At the user's option, the Rosin-Rammer distribution (Eq. 4.7.10) may be used to determine the distribution of droplet diameters.

The second major task is integrating the droplet equations and calculating the droplet collision interactions. Subroutine TRACK performs this calculation for one time step. The flow chart for TRACK is given on Fig. 8.2 which shows the breakdown of the major task into eight smaller tasks. At the beginning of each station on the course grid (J station) IPR=1, the droplet data is read from unit KTDRUM and the flow field variables from unit NDRUM. For each step on the fine grid (JKDS>1) and IPR \neq 0, and the flow field and coordinate variables are interpolated.

The droplet class is defined by the index IJK calculated from the nested D \emptyset loop indices. Thus for each droplet, the droplet motion is calculated by PARPAT, a determination is made if the droplet hits a boundary by WALLRB, and depending on the options I \emptyset PT1 and IBREK, a determination is made on whether the droplet shatters by BREKUP, and whether the droplet is a member of the two largest classes by L \emptyset CGRD. When the solution for all the droplets at the new time step is determined, L \emptyset GC \emptyset L examines the two largest classes and applies the collision model. The solution is then printed by subroutine PRINT and stored by subroutine SMTER.

The equations of droplet motion are contained in PARPAT which are integrated for one time step using the predictor corrector method described in Section 4.11. Table 8.1 shows a breakdown of the tasks performed by PARPAT. FINTP locates the droplet on the computational grid and interpolates the flow field variables at that point. FPR \emptyset P, GPR \emptyset P, and PPR \emptyset P calculates the thermodynamic and transport properties for the film, air, and, liquid respectively. DIFFUS calculates the mass diffusion coefficient (Eq. 4.4.16), P \emptyset LY is a polynomial interpolation, C \emptyset XCH is the Cox chart (see Section 4.5). DRAGF contains the drag coefficient correlation (Eq. 4.2.8) and NUSSET contains the Nusselt number correlations (Eqs. 4.4.1, 4.4.2) for heat and mass transfer. VAHR calculates the heat and mass transfer rates (Eqs. 4.3.4 and 4.3.1). The equations of motion (Eqs. 4.2.1 through 4.2.6) are programmed directly

using DRAGF. The role of change of droplet temperature (Eq. 4.3.3) and droplet diameter (Eq. 4.3.9) is calculated by DTEMP and DDIAM respectively. When the predictor corrector iteration converges (Eq. 4.11.10) the time step is known and the calculation of critical species is made. X2INIT calculates the initial distribution of critical species in the film surrounding the droplet. X2INIT requires VAHR and PFILM to calculate the local partial pressure. XX2 integrates the rate equation (Eq. 8.3.1) using XRATE. X2MASS integrates over the film volume to obtain the mass of critical species (see Eq. 8.2.6). Finally the total heat input to the droplet (see Eq. 8.2.11) is calculated.

The third task in TRACK (Fig. 8.2) is to examine the droplet to see if it hits a boundary using subroutine WALLRB. For purely elastic wall rebound, the velocity component normal to the wall is changed in sign. For periodic boundary conditions, a droplet leaving one boundary enters on the opposite boundary. A portion of the droplets may stay on the wall and form a liquid film. These conditions are calculated by subroutine BOUNCE. BOUNCE determines the fraction of droplets that remain on the wall using the models described in Section 4.10. Of the fraction that remains on the walls, some portion will evaporate depending on the wall temperature and partial pressure calculated from the Cox chart using subroutine COXCHT as described in Section 4.10.

The next step is to determine if a droplet shatters using subroutine BREKUP and the models described in Section 4.9. The droplet shattering model is applied to all classes. After shattering the droplets are counted with the nearest class rather than forming new classes. However, the two largest classes in each computational grid must be recalculated using L0CGRD.

Once the new droplets conditions are established for all classes (IJK loop completed), the droplet collision model L0GC0L can be applied. L0GC0L searches through the computational grid and determines if the two largest classes are in the same grid volume. If they are in the same grid volume, subroutine C0LLDE determines if a collision occurs, and the conditions after a collision using the model described in Section 4.8. A fraction of the droplets may coalesce and a fraction may rebound with elastic collisions. Of those that rebound, subroutine C0LLSN calculates the approach velocity along the line of centers and subroutine C0LDYN calculates the rebound velocity. Subroutine C0LLSN contains the velocity transformation matrix and its inverse to go from the computational coordinates to the collision coordinates. Following the collision, the new properties of the classes are calculated in C0LLDE. The solution is printed by PRINT and stored on files NBQUND,ISDRV,KTDRUM, by SMTER at each Jth station of the course computational grid. This last step completes the calculation in TRACK.

Returning to PTRAK, Fig. 8.1, the calculation continues until the outer D0 loop is completed. An output summary is printed for all J stations on the course grid by subroutine SUMRY. Depending on the input option I0PT7, the source terms are calculated by DATAM. DATAM searches through all the solution files and calculates

the source terms \dot{W}_f and $\dot{W}_{f,w}$ for the vapor diffusion equation (Eq. 5.2.1) using Eqs. 4.7.14 and 4.7.15. This result is stored on file MDRUM. It then calculates the source term S_d for the critical species equation (Eq. 8.2.1) using Eq. (8.2.6) and stores the result on file MDRUM1. Finally it calculates the temperature drop due to evaporation and stores the results on file MDRUM2. At this point the calculation in PTRAK is complete.

FLOW CHART FOR SUBROUTINE TRACK

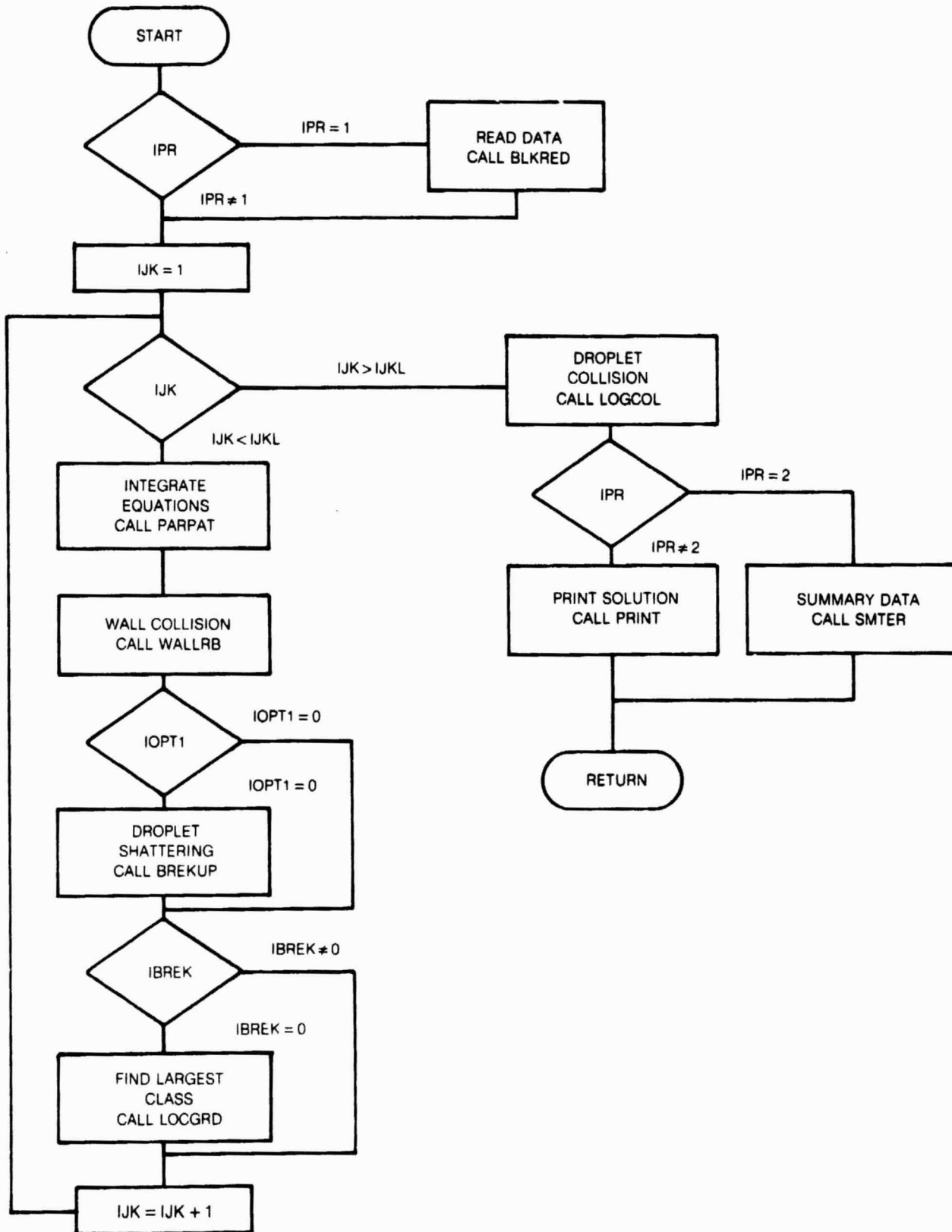


Table 8.1

Tasks in Subroutine PARPAT

| Subroutine | Task | Aux. Subroutines |
|-------------------------|--|-------------------------------|
| FINTP | locate droplet on grid find local air flow conditions | |
| FPRØP GPRØP PPRØP | film properties (Eqs. 4.4.6 to 4.4.20) air properties liquid properties (Eqs. 4.4.21 to 4.4.28) | DIFFUS PØLY POLY, CØXCH |
| DRAGF NUSSET | drag coeff. (Eq. 4.2.8) Nusselt No. (Eq. 4.4.1, 4.4.2) | |
| VAHR | determine heat transfer (Eq. 4.3.4) determine mass transfer (Eq. 4.3.1) Equations of motion (Eqs. 4.2.1 to 4.2.6) | |
| DTEMP DDIAM | Rate of temperature change (Eq. 4.3.3) Rate of diameter change (Eq. 4.3.9) | |
| X2INIT XX2 X2MASS | Initialize critical species Integrate rate equation (Eq. 8.3.1) Integrate mass (bracket Eq. 8.2.6) Integrate bracket (Eq. 8.2.11) | VAHR, PFILM PFILM, XRATE |

8.3 List of Subroutines in PTRAK

| | |
|--------|---|
| ALJPØT | Evaluate Leonard Jones Potential collision integral |
| BLKDAT | Block data |
| BLKRED | Read/Write data on files |
| BØUNCE | Wall rebound model |
| BREKUP | Droplet Shattering model |
| CØLDYN | Calculate droplet velocity after collision |
| COLLDE | Droplet Collision model |
| CØLLSN | Calculate velocity transformation matrix |
| CØØR | Read coordinate data |
| CØXCHT | Determine vapor pressure from Cox chart |
| DATAM | Store fuel sources for VAPDIF |
| DDIAM | Calculate rate of change in droplet diameter |
| DIFFUS | Calculate mass diffusivity |
| DISTEM | Determine distillation temperature |
| DRAGF | Calculate droplet drag |
| DTEMP | Calculate rate of change of droplet temperature |
| FBIN | Calculate binomial distribution |
| FINTP | Interpolate flow field of air |
| FNØZ | Calculate initial conditions for droplets |
| FPRØP | Determine fluid properties of film |
| GAMFUN | Calculate Gamma function |
| GPRØP | Determine gas properties for droplet |

| | |
|---------|--|
| INPUT | Read Input data |
| INITIAL | Initialization of particle classes |
| L0CGRD | Determine two largest classes |
| L0GC0L | Logic for Droplet collision model |
| L00K | Interpolation for table lookup |
| NUSSET | Calculate Nusselt number |
| 0UTPUT | Write initial input conditions |
| PARPAT | Integrate particle path equations |
| PFILM | Calculate local film properties |
| P0LY | Perform polynomial curve fit |
| PPR0P | Determine fluid properties of droplets |
| PRINT | Print class properties at each station |
| PTRAK | Main program |
| SMTER | Calculate summary terms |
| SUMRY | Write summary output |
| TRACK | Track droplet particle classes |
| VAHR | Calculate heat and mass transfer rates |
| WALLRB | Logic for wall rebounds |
| XRATE | Calculate net production of X_2 |
| XX2 | Calculate X_2 for one time step |
| X2INIT | Initialize X_2 mole concentration |
| X2MASS | Calculate mass of X_2 in droplet |

8.4 List of COMMON BLOCK Variables

The COMMON BLOCK variables are grouped into labeled COMMON BLOCKS. Alphabetical listing is by labeled COMMON BLOCK name. The COMMON BLOCK name is given and a general description of the variables in the group. Following this is a detailed list of variables in the order in which they appear in the COMMON BLOCK. COMMON BLOCK variables for the ADD code are given in Ref. 4.

| COMMON/ACONS/ | ADD Code Variables (Ref. 4) | |
|---------------|-----------------------------|---|
| COMMON/APART/ | Droplet Input Conditions | |
| RNZCLI(N,1) | r | Injector radius (cm) |
| RNZCLI(N,2) | z | Injector axial location (cm) |
| RNZCLI(N,3) | ϕ | Injector circumferential location (rad.) |
| RNZI(N) | | Radial displacement of r (cm) |
| ALPHI(N) | α | Angle between normal and streamwise (deg) |
| BETAI(N) | β | Angle between tangential and streamwise (deg) |
| VMEANI(N) | V | Magnitude of velocity (M/sec) |
| DPRTI(N) | D_L | Mean diameter of droplet (micron) |
| DDPRTI(N) | δD_L | Variance of droplet diameter (micron) |
| NNØZ | | Number of ejectors |
| DALP(N) | $\delta\alpha$ | Variance in α (deg) |
| DBET(N) | $\delta\beta$ | Variance in β (deg) |
| ILØC | | Number of ejectors |
| IVS | | Number of velocity classes |
| IPHI | | Number of α classes |
| ITHE | | Number of β classes |
| IDIA | | Number of droplet diameter classes |
| DVMI(N) | δV | Variance of Mean Velocity |

COMMON/BONVAR/ Crossection Boundary Variables

| | | |
|--------------|--------------|------------------------------------|
| C1,C2 | | Wall rebound probability constants |
| RTIP | r_H | Tip radius (cm) |
| RHVB | r_T | Hub radius (cm) |
| LPHI | | Number of ϕ grid point |
| DPHI | $\Delta\phi$ | Increment in ϕ (rad) |
| LPART | | Index in ϕ |
| PHIL | ϕ_L | Left ϕ boundary (rad) |
| PHIR | ϕ_r | Right ϕ boundary (rad) |
| RPART(L,1) | $r_t(\phi)$ | Tip boundary (cm) |
| RPART (1,2) | $r_H(\phi)$ | Hup boundary (cm) |
| PHPART (K,1) | $\phi_L(r)$ | Left & boundary (rad) |
| PHPART (K,2) | $\phi_r(r)$ | Right & boundary (rad) |

COMMON/BPART/ Droplet Input Thermodynamic Properties

| | | |
|-----------|----------|--|
| RHØLPI(I) | ρ_L | Droplet density (gm/cm ³) |
| TEMP(I) | T_L | Droplet temperature (°K) |
| DLP(I) | D_L | Droplet diameter (micron) |
| KPART(N) | | Radial index for N th droplet |
| PERLØC(I) | P_L | Percentage of fuel |
| JPLL | | |

COMMON/CARRAY/ Thermodynamic Polynomial Coeff.

| | | |
|-------------|----------------|---------------------------------------|
| CØEFP(1,I) | A _I | Droplet density (gm/cm ³) |
| CØEFP(2,I) | A _I | Droplet heat capacity (cal/cm/°K/sec) |
| CØEFP(3,I) | A _I | Droplet viscosity (gm/cm/sec) |
| CØEFP(4,I) | A _I | Gas heat capacity (cal/gm/°K) |
| COEFP(5,I) | A _I | Gas conductivity (cal/cm/°K/sec) |
| CØEFP(6,I) | A _I | Gas Viscosity (gm/cm/sec) |
| CØEFP(7,I) | A _I | Air heat capacity (cal/gm/°K) |
| COEFP(8,I) | A _I | Air conductivity (cal/cm/°K/sec) |
| CØEFP (9,I) | A _I | Air viscosity (gm/cm/sec) |

$$F(T) = \sum_{I=1}^4 A_I T^{I-1}$$

COMMON CCRATE Parameters for Critical Species

| | | |
|-------------|--|---|
| AB, AF | A _b , A _f | } Constants in rate equation (Eq. 8.3.1) |
| EB, EF | E _b , E _f | |
| ALPB, ALPF | α _b , α _f | |
| BETB, BETF | β _b , β _f | |
| GAMB, GAMF | γ _B , γ _B | |
| CARBN | δ | |
| MOLE1,MOLE2 | M ₁ ,M ₂ | Molecular weights |
| BRAD | (r _d +b)/r _d | Film thickness ratio |
| YO2 | Y _{O2} | Mole fraction of O ₂ |
| DELM2 | (X ₂ /X ₁) ₀ | Initial ratio |
| LRLP | | Number of points in film |

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| | | |
|-------------|---------------------|-----------------------------|
| DELTB,DELTF | $\delta_b \delta_f$ | Constants for rate equation |
| ANUB,ANUF | $v_b v_f$ | (Eq. 8.3.11) |

COMMON /CCX21/ Mole Concentration Critical Species

| | | |
|----------|------------------------|---|
| X21 | $X_2(t)$ | Mole concentration (mole/cm ³) |
| X22(I) | $X_2(t+\Delta t)$ | Mole concentration (mole/cm ³) |
| DX2DO(I) | $(dX_2/dt)_{t+\Delta}$ | Production of X_2 (mole/cm ³ /sec) |
| DX2DT(I) | $(dX_2/dt)_t$ | Production of X_2 (mole/cm ³ /sec) |

COMMON /COLLVA/ Index for Largest Class

| | |
|--------------|--------------------------------|
| KGEØM(K,L,1) | Index for largest class |
| KGEØM(K,L,2) | Index for second largest class |

Where K = r grid index
L = ϕ grid index

COMMON /CONST/ ADD Code (Ref. 4)

COMMON /CONVER/ Constants

| | | |
|--------|---|---|
| GC | g | Force equivalent of mass (1.01325x10 ⁶ dyn/cm/atm) |
| JCØNST | J | Energy equivalent of work (41.311cm ³ mole/atm/°K) |
| RØCØN | R | Universal Gas Constant (82.087 cm ³ atm/mole/°K) |
| RØCØNP | R | Universal Gas Constant (1.98717 cal/mol/°K) |

COMMON /CORE/ ADD Code (Ref. 4)

COMMON /CORE2/ ADD Code (Ref. 4)

COMMON /COXCUR/ Cox chart data

| | | |
|-------|-------|------------------------|
| ICØX1 | | Number of input points |
| PICH | P_1 | Vapor pressure (atm) |

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| | | |
|--------------|--------|--|
| P2CH | P_2 | Vapor pressure (atm) |
| CØXCAR(1, I) | η | Carbon number |
| CØXCAR(2, I) | T_1 | $(T(\zeta, P_1))$ ($^{\circ}\text{K}$) |
| CØXCAR(3, I) | T_2 | $T(\zeta, P_2)$ ($^{\circ}\text{K}$) |

COMMON /CPART/ Dependent droplet variables

| | | |
|-------------|--------|--|
| PART(I, 1) | U_s | Streamwise velocity (m/sec) |
| PART(I, 2) | U_t | Tangential velocity (m/sec) |
| PART(I, 3) | U_n | Normal velocity (m/sec) |
| PART(I, 4) | n | Normal coordinate |
| PART(I, 5) | ϕ | Circumferential coordinate |
| PART(I, 6) | D_L | Droplet diameter (micron) |
| PART(I, 7) | T_L | Droplet temperature ($^{\circ}\text{K}$) |
| PART(I, 8) | r | Droplet radius (cm) |
| PART(I, 9) | z | Droplet axial distance (cm) |
| PART(I, 10) | t | Droplet time (sec) |
| PART(I, 11) | f | Probability |
| PART(I, 12) | M_2 | Mass of critical species (gm) |
| PART(I, 13) | Q | Total heat load (cal) |

COMMON /CURVE/ Distillation curve

| | | |
|--------------|-------|------------------------------------|
| IDSTIL | | No. of data points |
| DISCUR(1, I) | P_e | Percent evaporated |
| DISCUR(2, I) | T_b | Temperature ($^{\circ}\text{K}$) |

COMMON /DRED1/ ADD code (Ref. 4)

COMMON /DSKLOC/ ADD code (Ref. 4)

COMMON /DUCOUT/ ADD code (Ref. 4)

COMMON /DUCTIN/ ADD code (Ref. 4)

COMMON /FILVAR/ Film thermodynamic properties

| | | |
|--------|-----------------------|--|
| MF | M_m | Film molecular weight |
| RHOF | ρ_m | Film density (gm/cm ³) |
| CPF | C_{pm} | Film heat capacity (cal/gm/°K) |
| KF | k_m | Film thermal conductivity (cal/cm/°K/sec) |
| MUF | μ_m | Film viscosity (gm/cm/sec) |
| DMASSF | m | Film mass diffusivity (cm ² /sec) |
| CFE | C_f | Fuel mass fraction |
| CGF | C_a | Air mass fraction |
| SIGP6F | σ_m | Film force constant (A) |
| OMEGF | Ω^* | Collision integral |
| YINF | Y_∞ | Air mole fraction |
| YGF | $1-Y_m$ | Average film air mole fraction |
| YPF | Y_m | Average film fuel mole fraction |
| YPSF | $Y_{f,s}$ | Fuel mole fraction at droplet surface |
| CKPGF | $(\epsilon/\kappa)_m$ | Force constant film (°K) |
| TSTARF | T^* | Dimensionless temperature |
| YPINF | $Y_{f,\infty}$ | Mole fraction of air at film edge |
| MINF | M_a | Molecular weight air |

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COMMON /FLAGS/ ADD code (Ref. 4)

COMMON /FUNC/ ADD code (Ref. 4)

COMMON /GASVAR/ Gas thermodynamic properties

| | | |
|------|-----------------------|---|
| MG | M_a | Air molecular weight |
| PCG | P_{ca} | Air critical pressure (atm) |
| TCG | T_{ca} | Air critical temperature ($^{\circ}$ K) |
| SIGG | G_a | Air force constant (\AA) |
| CKG | $(\epsilon/\kappa)_a$ | Air force constant ($^{\circ}$ K) |
| CPG | C_{pa} | Air heat capacity (cal/gm/ $^{\circ}$ K) |
| KG | k_a | Air thermal conductivity (cal/cm/ $^{\circ}$ K/sec) |
| MUG | μ_a | Air viscosity (gm/cm/sec) |

COMMON /INTINP/ Input Flags

| | |
|--------|------------------------------|
| KL | No. of streamlines |
| JL | No. of streamwise stations |
| KDS | No. steps/course grid |
| KLL | Not used |
| NB | Not used |
| ISHAPE | Not used |
| IØPTN | Input option see Section 5.2 |

N = 1,17

COMMON /MASSD/ Source terms for VAPDIF code

| | | |
|----------------|-----------------------|------------------------------|
| AMASS(K,L) | $w_f, S_d, \Delta T,$ | Source terms for VAPDIF |
| RDUM(K, ISIDE) | $w_{fw},$ | Wall source terms for VAPDIF |

| | | | |
|----------|--------------|---|---------------------------------|
| APARM(1) | $\Delta\phi$ | , | Circumferential step size (rad) |
| APARM(2) | LPHT | , | No. circumferential steps |
| APARM(3) | W_{fv} | , | Weight flow fuel (gm/sec) |
| APARM(4) | W_{fa} | , | Weight flow air (gm/sec) |
| APARM(5) | JLAST | , | Number of blocks |
| APARM(6) | I ϕ PT3 | , | input option |
| APARM(7) | JC ϕ UN | , | Block routine |

COMMON /MISCEL/ Miscellaneous variables

| | | | |
|-------------|-------|--|-----------------------------------|
| VEL | V | | Air velocity (m/sec) |
| TEMG | T_a | | Air temperature ($^{\circ}$ K) |
| PRESG | P_a | | Air pressure (atm) |
| RH ϕ G | P_a | | Air density (gm/cm ³) |

COMMON /NUMDEN/ Droplet Summary

| | | | |
|-----------|---------------------------|--|--|
| FMASS | $\overset{\circ}{W}_L$ | | Fuel flow rate (gm/sec) |
| FSUM | N_T | | No. fuel droplets/sec (1/sec) |
| SMDD | | | SMD denominator |
| SMDN | | | SMD numerator |
| SMD | SMD | | Sauter mean diameter (microns) |
| QF | $\overset{\circ}{W}_L$ | | Liquid fuel flow rate (gm/sec) |
| QFO | $\overset{\circ}{W}_{LO}$ | | Initial liquid fuel flow rate (gm/sec) |
| SARRAY(1) | z | | Axial location (cm) |
| SARRAY(2) | SMD | | Sauter mean diameter (micron) |
| SARRAY(3) | | | % fuel liquid |

| | |
|-----------|-------------------------------|
| SARRAY(4) | % fuel at wall that is liquid |
| SARRAY(5) | % fuel at wall that is vapor |
| SARRAY(6) | % fuel in vapor state |
| SARRAY(7) | % fuel evaporated |
| SARRAY(8) | Flow rate of vaporized fuel |
| SARRAY(9) | Fuel/Air ratio |

COMMON /NUSVAR/ Nusselt number variables

| | | |
|-----|--------|------------------------------|
| NUH | Nu_h | Nusselt number heat transfer |
| NUM | Nu_m | Nusselt number mass transfer |
| REN | Re_D | Reynolds number of droplet |
| PRN | Pr | Prandtle number |
| SCN | Sc | Schmidt number |

COMMON /PARVAR/ Droplet thermodynamic properties

| | | |
|-------|-----------------------|--|
| MP | M_L | Molecular weight fuel |
| TCP | T_c | Critical temperature of fuel ($^{\circ}K$) |
| PCP | P_c | Critical pressure of fuel (atm) |
| SIGP | σ_L | Force constant (\AA) |
| CKP | $(\epsilon/\kappa)_L$ | Force constant ($^{\circ}K$) |
| LAMBP | λ_L | Heat of vaporization (cal/gm) |
| SP | S | Surface tension (dyne/cm) |
| PVP | $P_{f,s}$ | Vapor pressure fuel (atm) |
| TMP | T_m | Film temperature ($^{\circ}K$) |
| RHØLP | ρ_L | Fuel liquid density (gm/cm ³) |
| CPLP | C_{PL} | Fuel liquid heat capacity (cal/gm/ $^{\circ}K$) |

| | | |
|------|----------|---|
| MULP | μ_L | Fuel liquid viscosity (gm/cm/sec) |
| CPVP | C_{pv} | Fuel vapor heat capacity (cal/gm/°K) |
| KVP | k_v | Fuel vapor thermal conductivity (cal/cm/°K/sec) |
| MUVP | μ_v | Fuel vapor viscosity (gm/cm/sec) |

~~COMMON~~ /QMON/

| | | |
|----------|----------------|---|
| QOLD(I) | \dot{q}_{si} | Heat transfer rate (cal/sec) |
| DMDTO(I) | $(dm_2/dt)_i$ | Mass rate of change of critical species |

~~COMMON~~ /REALIN/ ADD code (Ref. 4)

~~COMMON~~ /SVARB/ ADD code (Ref. 4)

8.5 List of Local Variables

A list of selected local variables appears below. These variables are alphabetically listed by subroutine name.

ALJPOT

TS T^* , Dimensionless temperature

ALJPOT Ω^* , Collision integral

BLKDAT ADD code (Ref. 4)

BLKRED ADD code (Ref. 4)

BOUNCE

IJK Class index

IBOUN Wall index

SP S Surface tension (dyne/cm)

TEMMIN Minimum droplet temperature ($^{\circ}$ K)

TEMMAX Maximum droplet temperature ($^{\circ}$ K)

ND N_T Number of droplets (1/sec)

PRB Probability of wall rebound

WFCOLL Amount of fuel/area (gm/cm^2)

WFEVDP Amount of fuel evaporated/area (gm/cm^2)

WFEVAT Total fuel evaporated (gm)

WFLIQT Total fuel on wall (gm)

BREKUP

IJK Droplet class index

IPREK Flag indicates shattering

A, B Constant Wolfe, Anderson shattering model

AK1, AK2 Aerodynamic drag constants

| | | |
|-------------------|------------------------|---|
| CD | C_D | Drag coefficient $C_D=1$ |
| DK3 | | Shattering Model constants DK3=136 |
| FK1,FK2 | | Friction drag constants FK1=2, FK2=4 |
| RHØLP | ρ_L | Density of droplet (gm/cm^3) |
| SP | S | Surface tension (dyn/cm) |
| VEL | $ V $ | Absolute velocity (m/sec) |
| DSHAT | | Droplet diameter after shattering (micron) |
| ND | N_T | Total number density after shattering (1/sec) |
| TEST1 | | Time of aerodynamic breakup (sec) |
| TEST2 | | Time of friction breakup (sec) |
| <u>CØLDYN</u> | | |
| IP1,IP2 | | Index for colliding classes |
| VEL11,VEL12,VEL13 | \vec{V}_J | Velocity after collision (V_s, V_n, V_ϕ) (m/sec) |
| VEL21,VEL22,V23 | \vec{V}_k | Velocity after collision (V_s, V_n, V_ϕ) (m/sec) |
| AMASS1,AMASS2 | m_J, m_K | Droplet mass before collision (gm) |
| E,EI | E, E^{-1} | Velocity transformation matrix |
| VCØL1,VCØL2 | \vec{V}_J, \vec{V}_K | Velocity in collision coordinates (m/sec) |
| UC1,UC2 | V_{CJ1}, V_{CK1} | Velocity before collision (m/sec) |
| VCL,VC2 | V_{CJ2}, V_{CK2} | Velocity after collision (m/sec) |
| <u>CØLLDE</u> | | |
| K,J | | Droplet index |
| RC | R_C | Distance between droplets (cm) |
| XC,YC,ZC | X_c, Y_c, Z_c | Relative coordinates (cm) |

COLLSN

| | | |
|------------|-----------------|--|
| IP1, IP2 | | Droplet index |
| XC, YC, Zc | X_c, Y_c, Z_c | Relative cartesian coordinates (cm) |
| A(I, J) | | Transform matrix streamline to cylindrical |
| B(I, J) | | Transform matrix cylindrical to cartesian |
| C(I, J) | | Transform matrix streamline to cartesian |
| D(I, J) | | Transform matrix cartesian to droplet |
| E(I, J) | E | Transform matrix streamline to droplet |
| EI(I, J) | E^{-1} | Transform matrix droplet to streamline |

CØØR

ADD code (Ref. 4)

CØXCHT

| | | |
|-------|-----------|----------------------|
| PRESS | P_v | Vapor pressure (atm) |
| BCØEF | β_n | Cox chart constants |
| TEMI | T_L | Droplet temperature |
| PERCT | P_c | Percent evaporated |

DATAM

| | |
|-------|---------------|
| IØP | Module switch |
| JCØUN | Block counter |

DDIAM

| | | |
|--------|----------------|--|
| WDØTSF | \dot{w}_L | Vaporization rate (gm/sec) |
| DRDT | $d(\rho_L)/dt$ | Rate of density change ($\text{gm/cm}^3/\text{sec}$) |
| DLP | D_L | Droplet diameter (micron) |
| DDIAM | $d(D_L)/dt$ | Rate of diameter change (micron/sec) |

DIFFUS

| | | |
|--------|-------|---|
| TEMP | T | Temperature (°K) |
| PINF | P_a | Air pressure (atm) |
| DIFFUS | | Mass diffusion coefficient (cm^2/sec) |

DISTEM

| | | |
|--------|-------|---------------------------|
| PER | P_e | Percent liquid evaporated |
| DISTEM | T_D | Distillation temperature |

DRAGF

| | | |
|-------|------------|---|
| RHØ | ρ_L | Droplet density (gm/cm^3) |
| DLP | D_L | Droplet diameter (micron) |
| TINF | T_a | Air temperature (°K) |
| PINF | P_a | Air pressure (atm) |
| VINF | V_i | Air velocity (m/sec) |
| VPART | V_i | Droplet velocity (m/sec) |
| VEL | ΔV | Relative velocity (m/sec) |
| CD | C_D | Drag coefficient |

DTEMP

| | | |
|-------|---------------------|-------------------------------------|
| QNET | $q_s - w_L \lambda$ | Net heat flux (cal/sec) |
| DLP | D_L | Droplet diameter (micron) |
| DTEMP | dT/dt | Rate of temperature change (°K/sec) |

FBIN

| | | |
|------|----------|-------------------------|
| IXX | | IXX th class |
| JXX | | Total number of classes |
| FBIN | f(I, IL) | Probability |

| | | |
|----------------|--------------------------------|-----------------------------------|
| <u>FINTP</u> | | |
| ANE | n | Normal coordinate |
| VV | | Metric coefficient |
| VS,VP | V_s, V_ϕ | Air velocity components (m/sec) |
| RØ | ρ_a | Air density (gm/cm ³) |
| TP | T_a | Air temperature (°K) |
| PS | P_a | Air pressure (atm) |
| RB,ZB | r,z | Coordinates of droplet (cm) |
| RSB,RNB | | Direction cosines of coordinates |
| VSΒ,VNB | | Curvatures of coordinates |
| KP | | Streamline index for droplet |
| M | | Index for solution variables |
| <u>FNØZ</u> | | |
| ANP | n | Normal coordinate |
| HEIT | H | Duct height (cm) |
| FL,FV,FT,FP,FD | $f_L, f_v, f_t, f_p,$ f_o | Probability functions |
| PF | ϕ | Circumferential location (rad) |
| RP,ZP | r,z | Droplet coordinates (cm) |
| VSP,VNP,VPP | V_s, V_n, V_p | Droplet velocity (m/sec) |
| <u>FPRØP</u> | | |
| PINP | P_a | Air pressure (atm) |
| <u>GAMFUN</u> | | |
| ARG | X | Argument |
| GAMFUN | $\Gamma(X)$ | Gamma Function |

GPROP

| | | |
|-----|----------|--|
| CPG | C_{pa} | Air heat capacity (cal/gm/°K) |
| KG | k_a | Air thermal conductivity (cal/cm/°K/sec) |
| MUG | μ_a | Air viscosity (gm/cm/sec) |

INPUT See Section 5.2

INITIAL See COMMON BLOCK variables

LOGGRD

IJK Index for droplet class

LOGCCL

| | | |
|----------|-----------------|--|
| X1,Y1,Z1 | X_J, Y_J, Z_J | Cartesian coordinates J^{th} droplet (cm) |
| X2,Y2,Z2 | X_K, Y_K, Z_K | Cartesian coordinates K^{th} droplet (cm) |
| XC,YC,ZC | X_c, Y_c, Z_c | Relative cartesian coordinates (cm) |
| RC | R_c | Distance along line of center (cm) |

LOOK

| | | |
|------|-------|--------------------------|
| X(I) | X_I | Table of abscissa values |
| Y(I) | Y_I | Table of ordinate values |
| XIN | X | Input abscissa |
| YOUT | Y | Output ordinate |
| KK | | Default flag |

NUSSET See COMMON /NUSVAR/

OUTPUT Self explanatory

PARPAT

| | | |
|---------------|--------------------|--|
| VS1, VN1, VP1 | V_s, V_n, V_ϕ | Droplet velocity components at t (m/sec) |
| AN1 | n | Normal coordinate at t |
| P1 | ϕ | Circumferential location at t (rad) |
| DLP1 | D_L | Droplet diameter at t (micron) |

| | | |
|---------------|----------------|--|
| TLP1 | T_L | Droplet temperature at t (°K) |
| VS2, VN2, YP2 | $V_s V_n \phi$ | Droplet velocity components t+dt (m/sec) |
| AN2 | n | Normal coordinate at t+dt |
| P2 | ϕ | Circumferential location t+dt (rad) |
| DLP2 | D_L | Droplet diameter at t+dt (micron) |
| TLP2 | T_L | Droplet temperature at t+dt (°K) |
| RB2, ZB2 | r, z | Droplet coordinates at t+dt (cm) |
| RHØLPO | ρ_{LO} | Initial droplet density (gm/cm ³) |
| DLPO | D_{LO} | Initial droplet diameter (micron) |
| KP | KP | Streamline index |
| DT2 | Δt | Time increment |
| QS1 | \dot{q} | Droplet heat transfer rate at t (cal/sec) |
| X2M2 | m_2 | Mass of critical species at t+dt (gm) |
| QHEAT1 | Q_1 | Total heat added to droplet at t (cal) |
| QHEAT2 | Q_2 | Total heat added to droplet at t+dt (cal) |
| DM1 | $d(m_2)/dt$ | Rate of change of mass at t (gm/sec) |
| <u>PFILM</u> | | |
| RL | r_L^{+b} | Droplet film radius (micron) |
| RLP | r_L | Droplet radius (micron) |
| TLP | T_L | Droplet temperature (°K) |
| PINF | P_a | Air pressure (atm) |
| PF | P_f | Vapor pressure fuel (atm) |
| TF | T_f | Temperature of fuel (°K) |
| XF | X_f | Mole concentration of fuel (mole/cm ³) |

FØLY

| | | |
|--------------|---------------------------------|---|
| I | | Property index |
| TEM | T | Temperature °K |
| <u>PPRØP</u> | | |
| TINF | T _a | Air temperature (°K) |
| TLP | T _L | Droplet temperature (°K) |
| DLP | D _L | Droplet diameter (micron) |
| RHØLPO | ρ_{LO} | Initial droplet density (gm/cm ³) |
| DPLO | D _{LO} | Initial droplet diameter (micron) |
| <u>PRINT</u> | | Self explanatory |
| <u>PTRAK</u> | | |
| FMC | | Conversion factor (cm/ft) |
| RHUB, ZHUB | r _H , z _H | ID wall coordinates (cm) |
| RTIP, ZTIP | r _T , z _T | OD wall coordinates (cm) |
| <u>SMTER</u> | | |
| WATR | \dot{W}_a | Weight flow air (gm/sec) |
| WFEVAT | | Weight flow gas (gm/sec) |
| WFLIQT | \dot{W}_L | Weight flow liquid droplets (gm/sec) |
| QF | \dot{W}_{LO} | Initial fuel flow (gm/sec) |
| z | z | Axial location (cm) |
| <u>SUMRY</u> | | Self explanatory |

TRACK

IDIA No. diameter classes
 ILØC No. location classes
 IPHI No. normal angle classes
 ITHE No. azimuthal angle classes
 IVS No. velocity classes
 IJK Class index

VAHR

QNET $q_s - w_s \lambda$ Net heat transfer rate (cal/sec)
 WØTSE w_L Vaporization rate (gm/sec)
 TLP T_L Droplet temperature (°K)
 DLP D_L Droplet diameter (micron)
 TINF T_a Air temperature (°K)
 PINF P_a Air pressure (atm)

WALLRB

IJK Droplet class index

XRATE

T T Temperature (°K)
 X1 X_1 Mole concentration species 1 (mole/cm³)
 X2 X_2 Mole concentration species 2 (mole/cm³)
 X02 X_{O_2} Mole concentration oxygen (mole/cm³)

XX2

| | | |
|------|------------|-------------------------------------|
| DLP1 | D_L | Droplet diameter at t (microns) |
| DT2 | Δt | Time step (sec) |
| TLP | T_L | Droplet temperature ($^{\circ}$ K) |
| PINF | P_a | Air pressure (atm) |
| TINF | T_a | Air temperature ($^{\circ}$ K) |

X2INIT

| | | |
|-------------------|-------|-------------------------------------|
| DLP | D_L | Droplet diameter (micron) |
| TLP | T_L | Droplet temperature ($^{\circ}$ K) |
| PINF | P_a | Air pressure (atm) |
| TINF | T_a | Air temperature ($^{\circ}$ K) |
| X2M2 | M_2 | Mass critical species (gm) |
| QIT \emptyset T | Q_L | Total heat added to droplet (cal) |

X2MASS

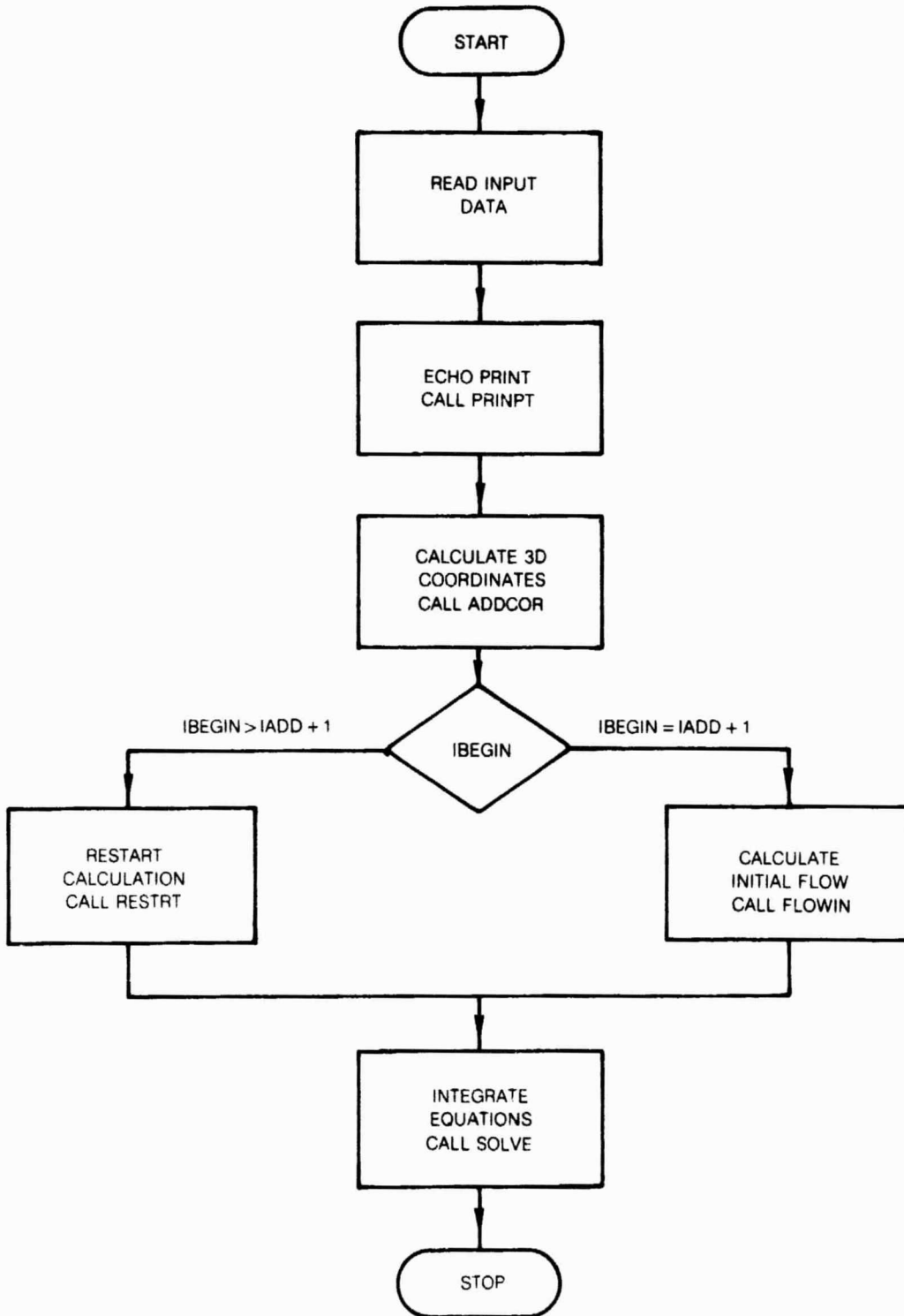
| | | |
|------------|-----------------|---|
| BRAD | $(r_d + b)/r_d$ | Film thickness ratio |
| DLP1, DLP2 | D_L | Droplet diameter at t Rt+dt (micron) |
| Dn2DT | dM_2/dt | Rate of mass change critical species (gm/sec) |
| DT2 | dt | Time step sec |

9.0 DETAIL DESCRIPTION OF VAPDIF CODE

9.1 Main Program/Flow Chart

The flow chart for the main program for the VAPDIF code is shown on Fig. 9.1. It consists of four major tasks: 1) Read and print the input data; 2) Calculate the three dimensional coordinates; 3) Calculate or restart initial conditions; and 4) Solve the diffusion equation. The run stream for execution of the code is given in Section 6.1. This run stream includes both input and output data files. A table of output file assignments is given on Table 7.3 and a table of unit numbers is given by Table 9.1. Table 9.1 shows both input and output files. NØP is the unit index used by the I/O routines. For input files the code generating the data is given by the code name in brackets. For output files the subroutine generating the data is given without brackets.

FLOW CHART FOR MAIN PROGRAM FOR VAPDIF



9.2 Description of Modules by Major Task

A complete list and brief description of all the subroutines is given in Section 9.3. The flow chart for the main program for VAPDIF is shown in Fig. 9.1 with an overall description given in Section 9.1. The description of the module functions will follow this flow chart. Only major tasks will be described. Input/Output routines are self explanatory and will not be described. Of the task shown on Fig. 9.1 only tasks two and four need be described.

Subroutine ADDCØR generates the three dimensional coordinate system used by the VAPDIF. Coordinates generated by the ADD code and stored on file 9, are read block by block. Each block corresponds to one streamwise station. ADDCØR then calculates the coordinates, metrics, and arc length distance and stores the result on unit 10. It then calculates the three dimensional cartesian coordinates for each mesh point and stores the results on unit 12. Finally it calculates the transformation matrix from the computational coordinates to the cartesian coordinates and stores the result on unit 13. Data on units 12 and 13 are not necessary for the solution but are useful for plotting results in physical space.

Subroutine SØLVE solves the diffusion equation (Eq. 5.2.1) or the critical species equation (Eq. 8.2.1) depending on the input option ISDG. The main program sets the first and last station. A flow chart for subroutine SØLVE is shown on Fig. 9.2. The first task is to align the data blocks on units 8, 17 and 28 with the absolute coordinate location of the coordinate grid stored on unit 9. The I DØ loop steps off streamwise stations from ILØW to INUM. Next flow field data calculated by the ADD code and stored on unit 8 is read and source terms stored on units 17 and 28 are read. The V DØ loop is an iteration loop for the point relaxation algorithm described in Section 5.1, and the K and J DØ loops sweep the entire crossplane grid including the boundary points. The coordinates stored on unit 10 are read by RDINB. The coefficients of the differential equations are calculated by CØEFFI. For ISDG>0, CØEFSG calculates the source term S_g for the critical species equation (Eq. 8.2.1). On the boundaries, PBNDC applies normal derivative boundary conditions, and PERBC applies periodic boundary conditions depending on the input options. PØISSN applies the difference operators (see Section 5.1) and solves for the v^{th} guess. With the completion of J, K grid sweep, a convergence check is made. If the solution converges, the solution is printed by PRDTSK and stores on unit 11 by WRØUT. The calculation then moves to the next station until the I DØ loop is completed. The calculation then returns to the main program.

FLOW CHART FOR SUBROUTINE SOLVE

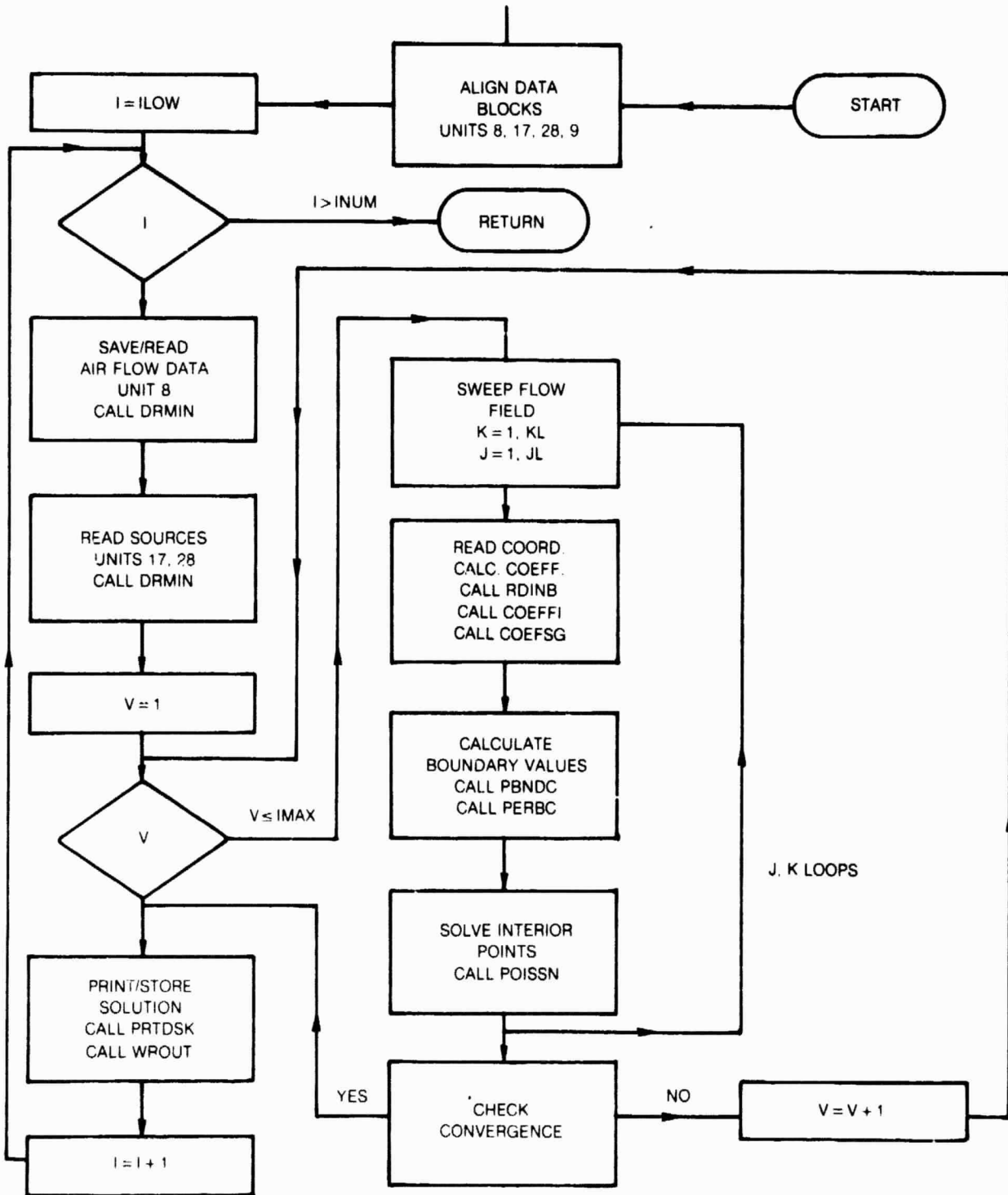


Table 9.1

Table of Unit Numbers

| NØP | NAME | UNIT | SUBROUTINE (CODE) | DATA |
|-----|--------|------|----------------------|--------------------------|
| 1 | IYDRM | 10 | ADDCØR | 3D coordinates |
| 2 | IFDRM | 11 | SØLVE | Output file |
| 3 | IXDRM | 12 | ADDCØR | 3D Castesian coordinates |
| 4 | ITDRM | 13 | ADDCØR | 3D transformation matrix |
| 5 | INDRM | 17 | (VAPDIF) | Mass fraction of fuel |
| 6 | IADDRM | 8 | (ADD) | Air flow field |
| 7 | ICØDRM | 9 | (ADD) | Axisymmetric coordinates |
| 8 | IFGDRM | 19 | (PTRAK) | Summary droplet data |
| 9 | 28 | 28 | (PTLAK) | Critical species source |

9.3 List of Subroutines in VAPDIF

| | |
|---------|---------------------------------------|
| ADDCØR | Calculate 3D coordinates |
| AINTG | Area integral of prescribed function |
| CØEFFI | Calculate coefficients of P.D.E. |
| CØEFSG | Calculate source for critical species |
| DERBDY | Calculate derivatives on boundaries |
| DERINT | Calculate interior derivatives |
| DERIV | Calculate derivatives |
| DFCØR | Correct fuel concentrate |
| DIFFUSE | Main program |
| DM2DT | Critical species rate equation |
| DRØUT | Input/Output module |
| FLØWIN | Initial conditions module |
| PBND | Neuman boundary conditions |
| PERBC | Periodic boundary conditions |
| PERIOD | Read boundary values |
| PØISSN | Solve Poisson's equation |
| PRINPT | Print module |
| PRUN | Metric conversion |
| PRTDSK | Print module |
| RDINA | Read contiguous block data |
| RDINB | Read overlapping block data |
| RESTRT | Restart module |

RB2-915362-40

| | |
|--------|--------------------------------------|
| RHØV | Integrand for flow integration |
| SØLVE | PDE solution algorithm |
| SØURCE | Integrand for area integral |
| SUMRY | Print summary data |
| WRØUT | Write contiguous block data |
| WRØUTB | Write overlapping block data |
| WTFLØW | Integrand of Mass flow area integral |

9.4 List of COMMON BLOCK Variables

The COMMON BLOCK variables are grouped into labeled COMMON BLOCKS. Alphabetical listing is by labeled COMMON BLOCK name. The COMMON BLOCK name is given and a general description of the variables in the group. Following this is a detailed list of variables in the order in which they appear in the COMMON BLOCK. COMMON BLOCK variables for the ADD code are given in Ref. 4.

COMMON /CADD/ ADD code Air flow variables (Ref. 4)

COMMON /CCRATE/ Variables for critical species rate equation

| | | |
|-------------|----------------------|------------------------------------|
| ISDG | | Option flag |
| SDG | S_g | Source of critical species |
| AB,AF | A_b, A_f | } Constants in Eq. 8.3.1 |
| EB,EF | E_b, E_f | |
| ALPB,ALPF | α_b, α_f | |
| BETB,BETF | β_b, β_f | |
| GAMB,GAMF | γ_b, γ_f | |
| CARBN | ζ | |
| RACONP | R | Gas constant (1.98717 cal/mole/°K) |
| MOLE1,MOLE2 | M_1, M_2 | Molecular weights |
| YO2 | Y_{O_2} | Mole fraction of O_2 |
| DELTB,DELTF | δ_b, δ_f | } Constants in Eq. 8.3.11 |
| ANUB,ANUF | ν_b, ν_f | |
| ISGMAX | | Flag |

COMMON /CF/ Dependent Variable

| | | |
|--------|-----------------|--------------------------------|
| F(J,K) | $f_{J,K}^{I-1}$ | Dependent variable at I-1, J,K |
|--------|-----------------|--------------------------------|

COMMON /CFE/ Coefficient of PDE

A2(J),A3(J) A_2, A_3 Coefficient of second derivative
 B2(J), B3(J) B_2, B_3 Coefficient of first derivative
 C(J) C Coefficient of function

COMMON /CFG/ Dependent Variable

GF(J,K) $f_{J,K}^I$ Dependent variable at I,J,K

COMMON /CFG2/ Mass fraction fuel

FG2(J,K) $C_{J,K}^I$ Mass fraction of fuel

COMMON /CMU/ Turbulent viscosity

XMUT(J) μ_T Turbulent viscosity (gm/cm/sec)

COMMON /CONV/ Conversion factors

FTCM 30.48 cm/ft
 LBKG .4538 lb/kg
 CKELRK 1.8 °R/°K
 FTM .3048 m/ft

COMMON /CT/ Coordinate transformation matrix

TCOR(L,M,J,K) $T_{I,J,K}^{L,M}$ Coordinate rotation matrix at I,J,K

COMMON /CX/ Cartesian coordinates

X(L,J,K) X_L Cartesian coordinate of point I,J,K

COMMON /CY/ Computational coordinates at I

Y(L,M,J,K)
 L = 1 Streamwise direction
 = 2 Principal normal direction
 = 3 Orthogonal direction

| | | |
|-------|---|---------------------------|
| M = 1 | Y | Coordinate at point I,J,K |
| = 2 | h | Metric (cm) |
| = 3 | y | Arc length (cm) |

COMMON /CYI/ Computational coordinates at I-1

YI(L,M,J,K) See COMMON /CY/

COMMON /DATABL/ I/O index data (see Table 9.1)

| | |
|--------------|------------------|
| INDX (NOP,1) | Unit number |
| INDX (NOP,2) | Block length |
| INDX (NOP,3) | Pointer location |
| INDX (NOP,4) | Not used |
| INDX (NOP,5) | |

COMMON /RESIDL/ Residuals

| | |
|--------|-----------------------|
| RES | Residual |
| IMAX | Max no. iterations |
| EPSLON | Tolerance |
| PCT | Percent change cutoff |
| RLX | Relaxation parameter |

COMMON /SAVC/ Solution variable on periodic boundary

| | | |
|----------|---------|---------------------------------|
| C2(J) | C(J,1) | Fuel mass fraction K=1 boundary |
| CKLMI(J) | C(J,KL) | Fuel mass fraction K=1 boundary |

COMMON /SAVF/ Air flow variables

FLDSAV(L,J) See ADD code

COMMON /SOURC/ Sources for fuel concentration equation

| | | |
|-------------|----------------|---|
| W(J,K) | \dot{w}_L | Source terms (gm/cm ³ /sec) |
| BDYY(L,M,J) | \dot{w}_{LW} | Wall source terms gm/cm ² /sec |
| WPARM(L) | | See COMMON/MASSD/ in PTRAK |

COMMON/SOURC2/ Sources for critical species equation

| | | |
|---------|-------|--------------------------------------|
| W2(J,K) | S_d | Source for critical species equation |
|---------|-------|--------------------------------------|

9.5 List of Local Variables

A list of selected local variables appears below. These variables are alphabetically listed by subroutine name.

ADDCOR (Ref. 4)

| | | |
|----------|---------------|---|
| Q(N,J) | | ADD code variables |
| ILA | | No. streamwise stations |
| JLA | | No. normal stations |
| IL,JL,KL | | No. mesh points in Y_1, Y_2, Y_3 directions |
| RADR | r_r | Reference length |
| DSTEP | Δs | Y_1 step size |
| DPHI | $\Delta \phi$ | Y_3 step size |

AINTC

| | | |
|-------|---|-----------------------|
| AINTC | | Area integral of f |
| I | | Axial station |
| FCN | f | Integrand of integral |
| FUNCT | | Dummy subroutine name |

CØEFF1 (Ref. 4)

| | | |
|--------------|----------|----------------------------------|
| F(INVAR,1,J) | | Air flow variables from ADD code |
| SCHM | Sc | Schmidt number |
| USR | u_r | Reference velocity |
| RHØR | ρ_r | Reference density |
| TEMPR | T_r | Reference temperature |
| VISCR | μ_r | Reference viscosity |

| | | |
|---------------|-------------|--|
| PRFSR | P_r | Reference pressure |
| DSTEP | Δs | Y_1 step size |
| <u>CØEFSG</u> | | |
| RØCØN | R | Gas constant (82.0575 cm ³ atm/mole/°K) |
| RØCØNP | R | Gas constant (1.9817 cal/mole/°K) |
| TINF | T_a | Air temperature (°K) |
| PJNF | P_a | Air pressure (atm) |
| UINF | U | Air velocity (m/sec) |
| X02 | X_{O_2} | Mole concentration of oxygen (mole/cm ³) |
| Y02 | Y_{O_2} | Mole fraction of oxygen |
| <u>DERBDY</u> | | |
| ID | | Direction index |
| IV | | Variable index |
| ITYPE | | Option |
| DIN | f | Input array (dependent variable) |
| I1,I2,I3 | | Dimensions of DIN |
| YIN | Y | Input array (independent variable) |
| JO,KO | | Smallest indices |
| DG | df/dy | First derivative |
| DDG | d^2f/dy^2 | Second derivative |
| B,A | | Intermediate values |

| | | |
|---------------|---|----------------------------------|
| <u>DERINT</u> | | See subroutine DERBDY |
| <u>DERIV</u> | | See subroutine DERBDY |
| <u>DFCØR</u> | | |
| WRATIO | | Fuel mass flow correction factor |
| <u>BIFFUS</u> | | |
| IADD | | Add code strating station |
| IBEGIN | | Starting station |
| IEND | | Ending station |
| <u>DM2DT</u> | | See COMMON /CCRATE/ |
| <u>DRØUT</u> | | |
| INUNIT | | Unit number |
| ADDR | | Output address |
| BLØCK | | Record length (words) |
| NMØVE | | Relative address |
| <u>FLØWIN</u> | | |
| CØNC | C | Initial mass fraction of fuel |
| <u>PBND</u> | | |
| AC,BC,CC,DC | | Coefficient PDE |
| BDYVAL | | Boundary value |
| J,K | | Mesh point |
| JJ,KK | | Sub block mesh point |
| JBDY | | Boundary index |
| SØLN | | Solution |

| | | |
|---------------|----------|---|
| <u>PERBC</u> | | See subroutine PBNDC |
| <u>PØISSN</u> | | |
| AC,BC,CC,DC | | Coefficients of PDE |
| JJ, KK | | Sub block mesh point |
| SØLN | | Solution |
| PRINTP | | See output format statements |
| <u>PRRUN</u> | | See COMMON/CONV/ |
| <u>PRTDSK</u> | | |
| IDX1, IDX2 | | Indices of variables |
| ISTAT | | Unit index |
| NØP | | Option |
| <u>RDINA</u> | | |
| I, J, K | | Mesh point index |
| JJ, KK | | Sub block index |
| ADDR1 | | Block length |
| NØP | | See Table 9.1 |
| <u>RDINB</u> | | See subroutine RDINA |
| <u>RESTR</u> | | |
| IBEGIN | | Starting station no. |
| <u>PHØV</u> | | |
| RH | ρu | Mass flux (slug/ft ² /sec) ✓ |
| <u>RLXCAL</u> | | |
| RLXCAL | | Relaxation parameter (Eq. 5.3.14) |

SOLVE

| | | |
|---------------|--------------|--|
| IADD | | ADD code station |
| IBEGIN, IEND | | Beginning/Ending station |
| J, K | | Mesh point |
| JJ, KK | | Sub block mesh point |
| ISIDE | | Boundary index |
| FTIL | f^{v+1} | Guess of solution |
| RES | | Residual |
| <u>SOURCE</u> | | |
| S | $\int_L h_1$ | Integrand |
| <u>SUMRY</u> | | See output format statements |
| <u>WRØUT</u> | | See subroutine RDINA |
| <u>WRØUTB</u> | | See subroutine RDINA |
| <u>WTFLØW</u> | | |
| WF | cpu | Mass flux fuel (slug/ft ² /sec) |

10.0 REFERENCES

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3. Anderson, O.L. and D.E. Edwards: Extensions to an Analysis of Turbulent Swirling Compressible Flow in Axisymmetric Ducts NASA contract NAS3-21853, UTRC Report R81-914720-18. February 1981.
4. Anderson, O.L, G.B. Hankins, D.E. Edwards: User's Manual for Axisymmetric Diffuser Duct (ADD) Code. NASA CR 165598, February 1982.