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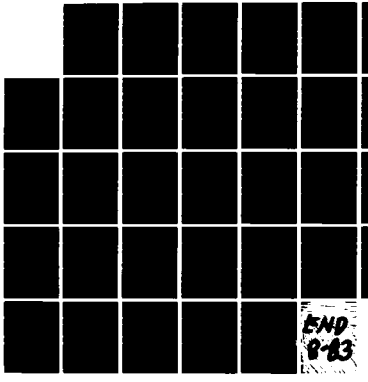

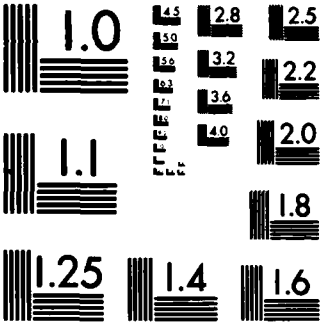

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REPORT SD-TR-83-27

The NEST Chemistry Computer Program: Operations Handbook

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This report has been reviewed by the Public Affairs Office (PAS) and is releasable to the National Technical Information Service (NTIS). At NTIS, it will be available to the general public, including foreign nationals.

This technical report has been reviewed and is approved for publication. Publication of this report does not constitute Air Force approval of the report's findings or conclusions. It is published only for the exchange and stimulation of ideas.

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Chemistry Computer Program	JANAF thermodynamic data
Equilibrium chemistry	Nonequilibrium chemistry
Flash photolysis	Quiescent gas
Frozen chemistry	Rocket performance
Incident and reflected shocks	Shock tube performance

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The NEST Chemistry Computer Program is used to calculate fluid and thermodynamic properties of frozen, equilibrium, and nonequilibrium chemically reacting one-dimensional flows. The operational procedure required for the use of the program is documented including detailed instruction for the preparation of input, a description of the output, and a typical deck setup for the running of production on The Aerospace Corporation's CDC 7600 or CYBER 176 computers.

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PREFACE

The authors gratefully acknowledge the helpful comments and suggestions, during the preparation of this report, of Drs. Norman Cohen, George R. Judd, Karl R. Westberg, and Roger L. Wilkins.

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TABLES

I. INTRODUCTION

The NEST (N-Element SysTem) computer program is used to calculate frozen, equilibrium, and nonequilibrium chemically reacting, steady, one-dimensional flow. NEST also can be used to calculate the variation with time of a stationary, reacting gas. The formulation of the equations and numerical methods used, the program structure, and input preparation are documented in Reference 1. The Holt-Gear-Newton implicit method of integration and the Emanuel-Aitken extrapolation integration method that are available in NEST are described in Reference 2.

In this report, the input preparation and output options are documented and some sample cases are presented to aid the NEST user. For questions regarding usage or chemical species available on the thermodynamic tape, contact Karen Foster.

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[1] E. B. Turner, G. Emanuel, and R. L. Wilkins, The NEST Chemistry Computer Program, Vol. I, TR-0059(6240-20)-1, The Aerospace Corporation (30 July 1970).

[2] W. D. Adams, et al., The RESALE Chemical Laser Computer Program, TR-0075(5530)-5, The Aerospace Corporation (20 February 1975).

II. INPUT DESCRIPTION

A. DATA STREAMS

The punched card input for the NEST computer program was designed to minimize input preparation errors and, at the same time, provide a format that is easy to recall and prepare. All input is punched free form in columns 1 through 70. Columns 71 through 80 are not used for the input program and can contain sequence numbers or other information.

The input consists of many data streams. A data stream is comprised of a keyword or keyword followed by a parameter field. The keyword identifies a function to be performed, and the parameter list contains the details of the task, e.g., the data stream that handles all print options that can be controlled by input is identified by the keyword PRINT. The parameter field for this data stream contains items such as the maximum number of answer stations to be printed. The character $ is reserved to denote the start of a data stream. The data stream can begin on any card, in any column, and continue through as many cards as necessary for completion of the stream.

The program searches the first data card for a $, which denotes the beginning of the first data stream. The search then continues through the card(s) for the next $, which denotes the beginning of the next data stream. Then, the function of the first data stream is determined by identifying the keyword, and the stream is passed to the area of the program that processes that particular function. The program continues in this manner until the end-of-case stream is encountered, at which time control is passed to an area that initializes the common storage area and calls in the appropriate computation overlay.

B. KEYWORD RULES

The purpose of the keyword is to identify that data stream. Keywords are up to 16 alphanumeric characters long and are chosen to indicate the function of the data stream. The keyword comprises the first nonblank characters following the $, but the keyword itself can contain imbedded blanks to improve

readability. For example, the keyword AREAVSX can be punched AREA VS X. If a parameter field follows, the keyword is terminated by either a comma or an equals sign. In the few data streams that do not contain a parameter field, the keyword is terminated by the start of a new data stream, i.e., the next $. The keywords are listed and described briefly in Table 1.

C. PARAMETER-FIELD CONSTRUCTION

The parameter field varies for different types of data streams. However, there are some general rules that might aid in constructing a parameter field. Information for setting up specific fields is presented in Section D. Each field consists of a collection of labels, species names, and numbers. A label is from 1 to 16 alphanumeric characters long, e.g., ATM or ROCKET, and is used to specify any number of options. Species names are from 1 to 12 nonblank alphanumeric characters and are generally written in standard chemical nomenclature (Table 2). Thus, gaseous species N_2, O, and F_2O are punched as N2, O, and F2O, respectively. Species in their vibrational states such as $H_2(v = 0)$ and HF (v = 10) are punched H2(0) and HF(10), respectively. A method of punching ionic species is to consider a pseudo element E as part of the molecule with a subscript denoting the charge in terms of loss or gain of electrons. In this notation, the three ionic species O_2^+, H^{-2}, and H_2O^{+3} in Table 2 become O2*E-1, H*E+2, and H2O*E-3. Condensed species such as water and solid carbon can be punched as H2O(L) and C (SOLID), respectively. Any nonnumeric information within the parentheses indicates a condensed species, not an excited species.

Numbers may be written in almost any way. For example, the following are equivalent: 3500, 3500., 3.5E+3, and +.35E4. The only rule is that if a number is written with an exponent, but with no decimal point, it is assumed that the decimal point precedes the first numeric, i.e., the number -2401E5 is equivalent to -.2401E+5.

Blanks in a parameter field are ignored; blanks can appear in species names, in numeric fields, and in labels to enhance readability without being considered part of the name, number, or label.

Table 1. Keyword and Data Stream Summary

Keyword	Function	Pg.	Keyword	Function	Pg.
TITLE	Problem title	12	G	Global catalyst	27
FLOW	Flow type description	13	T RATES	Rate temperature points	28
ATOMS	Atomic composition	15	STEP	Initial step size	28
QATOMS	Pseudo atoms	16	INTEG	Integration controls	29
P	System pressure	16	AREA VS X	Nozzle contour	30
T	System temperature	17	RADIUS VS X	Nozzle contour	31
RHO	System density	17	P VS X	Pressure contour	31
VEL	Flow velocity	17	RHO VS X	Density contour	31
H	System enthalpy	17	T VS X	Temperature contour	32
E	System energy	18	FLASH	Flashlamp constants	32
T RANGE	Temperature range	18	I VS T	Flashlamp output	33
P RANGE	Pressure range	18	PRINT	Print options	34
MOL/GM	Composition, mol/g	18	PLOT	Plot options	35
MOL PCT	Composition, mol %	19	SET GRID	Grid and scaling controls	39
WT PCT	Composition, wt. %	19	DUMP	Debug print options	43
MOL/CC	Concentration, mol/cm^3	19	V OBSERVER	Observer velocity	43
CHAMBER	Chamber conditions	19	FLAGS	Special controls	43
EXCITE	Excited system	20	END	End of case	46
INCL	Inclusion of species	20	NEW CASE	Begin new case	46
EXCL	Exclusion of species	21			
HEAT	Heat of formation update	22			
JANAF DATA	Thermodynamic data	22			
EQ	Chemical reaction	24			
KF	Forward rates	25			
KB	Reverse rates	26			
M	Catalyst	26			

Table 2. Species Name Input Convention

Species	Method Input
N_2	N2
O	O
F_2O	F2O
$H_2(v = 0)$	H2(0)
HF(v = 10)	HF(10)
O_2^+	O2*E-1
H^{-2}	H2*E+2
H_2O^{+3}	H2O*E-3
Solid C	C(SOLID)
Water	H2O (L)

D. DATA STREAM FORMATS

Each data stream must begin with a $ followed by one of the keywords listed in Table 1. If a parameter field is required, the keyword is followed by a separator (either a comma or an equals sign) and then the parameter field. Items in the parameter field are separated by either a comma or an equals sign.

Data streams can appear in any order in the input deck, except that the data streams in the compulsory category must appear before all others.

1. COMPULSORY

a. Case Title

This data stream contains a title to be printed at the top of each page of output. The stream begins with $TITLE = followed by a maximum of 72 characters ($ not permitted). Blanks are counted in the 72 character maximum.

Example: $TITLE = HF RUN NO. 92

b. Flow Type

The flow type is specified completely in this data stream. The keyword $FLOW = is followed by one or more flow labels. The acceptable flow labels are described in Tables 3 through 6.

Table 3. Nonequilibrium Flow Types

Flow Label	Remarks
SHOCK	Nonequilibrium shock tube performance is requested. This implies that the flow area is constant (flow area = 1 unless Flag 12 of Table 14 is input).
EXPAND[a]	Nonequilibrium expanding flow specified. A shape contour, either area or radius versus distance, must be input.[b]
P STREAM	Pressure streamtube performance is specified; a pressure contour must be input.[b]
RHO STREAM[c]	Density streamtube performance is specified; a density contour must be input.[b]
T STREAM	Temperature streamtube is specified; a temperature contour must be input[b]
Q GAS	The quiescent gas option applies. This option must be used with one of the above.

[a]Not necessary to specify throat position.
[b]The means of inputting contours is outlined in Subsection 8.
[c]Must use Q GAS with this flow type. This is flow type to use with flash lamp.

Example: $FLOW = RHO STREAM, Q GAS

Table 4. Frozen Equilibrium Shock Tube Flow Types

Flow Label	Remarks
INCIDENT	Calculate frozen and equilibrium conditions behind the incident shock.
REFLECTED	Calculate frozen and equilibrium conditions behind the reflected shock.
FFI	Calculate the frozen-frozen conditions behind the incident shock.
FFR	Calculate the frozen-frozen conditions behind the reflected shock.
FF/EQ	Calculate frozen-frozen incident; frozen-frozen reflected; frozen-equilibrium reflected; and frozen-frozen, equilibrium speeds, reflected cases only.

Example: $FLOW = FFI, FFR

Frozen-frozen incident and frozen-frozen reflected cases are to be calculated.

Table 5. Rocket and Wind Tunnel Flow Types

Flow Label[a]	Remarks
ROCKET	Rocket performance is specified. Use for unknown temperature. Input heat of formation.
WIND	Wind tunnel performance is specified. Use for pressure and temperature known.
EQ	Calculate equilibrium conditions.
FR	Calculate frozen conditions.
NONEQ	Calculate nonequilibrium conditions.

[a]Use $CHAMBER card.

Example: $FLOW = ROCKET, EQ, NONEQ

Equilibrium and nonequilibrium rocket performance are requested.

Table 6. Equilibrium Calculations

Flow Label	Remarks
GEN SOLVER	General solver, input a temperature and pressure range for which equilibrium conditions are to be found.
MOLLIER	Mollier tables are created for an input temperature and pressure range.
FLAME[a]	Compute a flame solution (rocket chamber combustion solution).
VOLUME[a]	Compute constant volume condition. Input pressure and density.

[a]Use $CHAMBER card.

Example: $FLOW = GEN SOLVER

c. Atomic Composition

The atomic composition of the system must be entered by means of this data stream. The keyword, ATOMS, is followed by a list of names of elements comprising the system. Table 7 contains the complete list of atoms recognized by the program. If ionized species are being considered, the pseudo element E must be included in the parameter list.

Example: $ATOMS = N, O, AR

The desired atomic composition consists of nitrogen, oxygen, and argon atoms.

Table 7. Element Names Set

H	NE	K	BR	CS
D	NA	CA	BR/81/	W
HE	MG	TI	KR	RE
LI	AL	CR	RB	PB
BE	SI	FE	ZR	BI
B	P	CJ (Cobalt)	MO	U
C	S	NI	CD	U/235/
N	S/34/	CU	SN	E (electron)
O	CL	ZN	I	
F	AR	BR/79/	XE	

d. Pseudo Atoms

Atoms not appearing in Table 7 can be included by means of the $QATOM data stream. The program will accept as an element name the letter Q followed by any letter in the alphabet. The enthalpy, entropy, and specific heat tables for the new atoms must be input by means of the $JANAF DATA stream. For this data stream, the keyword QATOMS is followed by the atom name, the base enthalpy, and the atomic weight of the atom. This data stream can be used in addition to the $ATOMS data stream.

Two new elements, QA and QB, are defined as follows:

$QATOMS, QA, 35, 1.5, QB, 32.56, 15.01

2. STATE VARIABLES

a. System Pressure

Keyword P is followed by the system pressure and one of the labels ATM, MM, or PSIA. The cold pressure follows if $CHAMBER is being used and mass flow is an input quantity.

Example: $P = 1500, ATM

System pressure is 1500 ATM.

$P = 837, MM, COLD = 500

System pressure is 837 Torr, and cold pressure is 500 Torr.

b. System Temperature

The system temperature, in degrees Kelvin, is set by keyword T followed by the desired temperature.

Example: $T = 2.98E2

c. System Density

The system density, in grams per cubic centimeter, is set by keyword RHO followed by the density. Note that if the system composition is input in moles per cubic centimeter, the program can be used to compute the system density and this data stream can be omitted.

Example: $RHO = 1.9E-4

d. Flow Speed

The flow speed, in centimeters per second, is determined by keyword VEL followed by the flow speed.

Example: $VEL = 54000

If the flow is one of the frozen-equilibrium shock types (see Table 4), a set of velocities in millimeters per microsecond for which the frozen-equilibrium conditions are to be calculated can follow in the parameter list.

Example: $VEL = 3, 2.5, 2, 1.5

Conditions are to be computed for velocities equal to 3, 2.5, 2, and 1.5.

e. System Enthalpy

The system enthalpy, in kilocalories per mole, is input by keyword H followed by the enthalpy value.

Example: $H = 3.93

f. System Energy

The system energy, in kilocalories per mole, is input by keyword E followed by the energy.

Example: $E = 4.9

g. Equilibrium Temperature Range

A temperature range must be specified for the general solver flow type. This is set by keyword T RANGE followed by an initial temperature, a final temperature, and a temperature decrement.

Example:

Answers at temperatures of 3000, 2500, 2000, and 1500 K are obtained by:

$T RANGE = 3000, 1500, 500

An answer at a single temperature point of 3000 requires the use of

$T RANGE = 3000, 3000, 0

h. Equilibrium Pressure Range

A pressure range (in standard atmospheres) must be set for the general solver flow type. This is accomplished by keyword P RANGE followed by an initial pressure, a final pressure, and a pressure decrement.

Example: $P RANGE = 2.8, 1.2, .4

3. COMPOSITION

a. Moles per System Gram

Keyword MOL/GM is followed by sets of species name and moles per gram for that species, respectively.

Example:

To input $.53 \times 10^{-3}$ mol/g of O_2, $.24 \times 10^{-1}$ mol/g of N_2, $.39 \times 10^{-2}$ mol/g of NO, $.252 \times 10^{-2}$ mol/g of N, and $.95 \times 10^{-2}$ mol/g of O, write

$MOL/GM, O2 = .53E-3, N2 = .24E-1, NO = .39E-2, N = .252E-2, O = .95E-2

b. Mole Percent

Keyword MOL PCT is followed by sets, each comprising a species name and its percent amount. The percent amounts must sum to 100%.

Example:

A composition of 1% water vapor and 99% argon is specified by

```
$MOL PCT, H2O = 1, AR = 99
```

c. Weight Percent

Keyword WT PCT is followed by sets each comprising a species name and its weight percent amount. The percent amounts must sum to 100%.

Example:

A composition of 96.3% fluorine and 3.7% carbon monoxide is specified by

```
$WT PCT, F2 = 96.3, CO = 3.7
```

d. Moles per Cubic Centimeter

Keyword MOL/CC is followed by sets, each comprising a species name and its concentration in moles per cubic centimeter. Note that when this data stream is used, the program can compute the system density so it need not be input.

Example: Concentrations of $.19 \times 10^{-2}$ of Cl_2, 3.8×10^{-6} of H_2, and 3.8×10^{-9} of H are set by

```
$MOL/CC, CL2 = .19E-2, H2 = 3.8E-6, H = 3.8E-9
```

e. Chamber Conditions

This data stream is used to specify the system composition for all rocket and wind tunnel flow cases, and the flame and constant volume equilibrium solutions. The keyword CHAMBER is followed by the chemical name of the species, an optional label for printout purposes, the heat of formation in kilocalories per mole (not required for wind tunnel cases), and the amount of the species being introduced followed by the label FUEL if the species is a fuel and the mixture ratio option is being used. In general, the data stream is as follows:

$CHAMBER, CHEM = name, LABEL = name, HEAT = number

MASS FLOW
MOL/GM
MOL PCT = number, CHEM = species, etc.
WT PCT
or MIX = number FUEL, CHEM = species, etc.

Example:

The system composition in moles per gram for a wind tunnel case may be set by:

$CHAMBER, CHEM = O2, MOL/GM = .539E-3, CHEM = N2, MOL/GM = .241E-1,
CHEM = NO, MOL/GM = .394E-2

A rocket case composition can be specified in mass flow (grams per second) as follows:

$CHAMBER, CHEM = HE, LABEL = HELIUM, MASS FLOW = 4.5,
CHEM = SF6, MASS FLOW = 2.8, CHEM = O2, MASS FLOW = .61

4. SPECIES SPECIFICATION

a. Excited Species Inclusion

Excited species are accepted in the system if $EXCITE (no parameter field is needed) is written.

b. Inclusion of Species

There are various ways to select the set of species that constitutes the total system for this data stream. These are described in the following subsections.

(1) Case 1

The system is not specified by input, i.e., data streams $INCL and $EXCL are not used. One of two selection methods is used in this situation.

(a) When an equilibrium or frozen calculation, or both, is required, the program selects from the thermodynamic data library tape all species with

atomic composition represented by the set of elements listed in the $ATOMS and $QATOMS data streams.

(b) When only nonequilibrium calculations are required, the system is composed of all species appearing on reaction cards, catalyst cards, and composition cards.

(2) Case 2, Inclusion of Species

The user has listed the system species in a $INCL data stream. One of two selection methods applies.

When an equilibrium or frozen calculation, or both, is required, the system is composed of all species in the $INCL stream. If the elements from $ATOMS are missing from this list, the program will add them to the system.

When only nonequilibrium calculations are required, the system will include all species in the $INCL stream plus any species that are not in the $INCL stream but appear in reaction, catalyst, or composition data streams.

This data stream begins with $INCL followed by species names separated by commas (or equal signs).

Example: $INCL = H, F, H2, F2, HF(0), HF(1)

(3) Case 3, Exclusion of Species

Species to be excluded from the system are listed in the $EXCL data stream, and the system is chosen in one of two ways.

When an equilibrium or frozen calculation, or both, is required, the program begins selecting species from the thermodynamic data library as in case 1(a), but excludes any species from the $EXCL data stream. If one of the elements from $ATOMS is present in the $EXCL list, its presence in $EXCL is ignored, and the element is included in the system.

When only nonequilibrium calculations are required, the system is chosen as in case 1(b), but any species in the exclude list are deleted. However, all species in reaction, catalyst, and composition data streams are included in the system even though they may appear (assumed incorrectly) in the $EXCL list.

The methods of selecting the species in the system, as outlined in the description of the preceding data stream, must be understood if this option is to be used. The data stream begins with $EXCL followed by a list of species to be excluded from the total system.

Example:

Assuming that O and C appear in the $ATOMS list, the following data stream could be used to exclude the indicated species:

$EXCL = CO2, C2, C3, C5

5. THERMODYNAMIC DATA

a. Heat of Formation Update

The thermodynamic library tape value for the heat of formation can be changed during a run by specifying the keyword HEAT followed by sets of a species name and a new value for the heat of formation.

Example: The heat of formation for OH and O3 can be set to 9.3 and 34.2, respectively, by writing $HEAT, OH = 9.3, O3 = 34.2.

b. Thermodynamic Data Update

This data stream can be used to change the thermodynamic data from the thermodynamic data tape for a system species and to provide data for a species not present on the tape. The thermodynamics of any species comprised of elements defined by the QATOMS option must be specified by this data stream. The keywords JANAF DATA are followed by the species name, the heat of formation, and a table containing temperature, molar heat capacity, enthalpy, and entropy. The temperature values must be a continuous subset of the temperature range on the tape (see Table 8). If a range of temperature values T is input such that $T_1 \leq T \leq T_2$, the program sets the thermodynamic data values for all $T < T_1$ equal to the values of T_1 and all values of $T > T_2$ equal to the values of T_2.

Example: $JANAF DATA, C2F2, HEAT = 5.1,
1000, 20, 12, 78.5,
1100, 20, 14, 80,

```
1200, 20, 15.9, 81.9,
C2, HEAT = 200.0, 1000, 8.582, 6.202, 58.524
QAO2, HEAT = -22.38, 1000, 23.338,
14.412, 89.935, 1100, 23.788, 16.769, 92.181
```

These input data update the thermodynamics for molecules C2F2, C2, and QAO2, as shown in Table 9. Note that since only one temperature was specified for C_2, all thermodynamic data for C_2 are set equal to the input data at T = 1000.

Table 8. Thermodynamic Table Temperature Range

0	1800	3900
50	1900	4000
100	2000	4100
150	2100	4200
200	2200	4300
250	2300	4400
298.15	2400	4500
300	2500	4600
400	2600	4700
500	2700	4800
600	2800	4900
700	2900	5000
800	3000	5100
900	3100	5200
1000	3200	5300
1100	3300	5400
1200	3400	5500
1300	3500	5600
1400	3600	5700
1500	3700	5800
1600	3800	5900
1700		6000

Table 9. Thermodynamic Data Update

Species C_2F_2		$\Delta HF^{\circ}_{298} = 5.1$	
T	C°_p	$H^{\circ}_T - H^{\circ}_{298}$	S°
1000	20	12	78.5
1100	20	14	80
1200	20	15.9	81.9

Species C_2		$\Delta HF^{\circ}_{298} = 200$	
T	C°_p	$H^{\circ}_T - H^{\circ}_{298}$	S°
1000	8.582	6.202	58.524

Species QAO_2		$\Delta HF^{\circ}_{298} = -22.38$	
T	C°_p	$H^{\circ}_T - H^{\circ}_{298}$	S°
1000	23.338	14.412	89.935
1100	23.788	16.769	92.181

6. REACTION DATA

a. Chemical Reaction

The reaction data stream is of the format $EQ XXX, chemical equation, where EQ XXX is the keyword portion followed by a chemical equation. The term XXX can be omitted or can be a maximum of three digits, representing a unique serial number for the reaction. This serial number is used for updating purposes only; if the rate constants for the reaction are not to be changed in succeeding cases, the serial number can be omitted.

The following rules must be observed when writing a chemical equation.

a. The reaction sign (⇌) is replaced by an equals sign (=).

b. A maximum of four species (not including catalysts) appears on each side of the equation.

c. If a catalytic species is involved, the catalyst appears, as does a species, on both sides of the equation, as MI, where I is an integer indicating which catalyst set is to be used. In this case, catalyst set I must be defined by a catalytic species data stream (Section 6d).

d. Global catalysts, if required, also appear as a species on both sides of the equation, as GI, where I is a global catalyst set defined by a global data stream catalyst set (Section 6e).

e. The user must terminate a species name with a comma, except when the species is the last species on either side of the reaction.

f. A species can appear only once on a side.

Examples:

(1) $O_2 + H_2 \rightleftarrows 2O + 2H$ (original)

O2, + H2 = 2O, + 2H (input version)

(2) $O_2 \overset{M_3}{\rightleftarrows} 2O$ (original)

O_2, + M3 = 2O, + M3 (input version)

In this example, catalyst set 3 must be defined by a catalyst data stream.

(3) $H_2O \rightleftarrows H_2O^+ + e$ (original)

H2O = H2O+, + E (input version)

or H2O = H2O*E-1, + E

(4) $C_3H_6O_3 + G1 \rightleftarrows CH_3CHO + CH_2OO + G1$ (original)

C3H6O3, + G1 = CH3CHO, + CH2OO, + G1 (input version)

Global catalyst 1 must be defined in a global catalyst data stream.

(5) H + H = 2H

This is unacceptable because it violates rule f.

b. Forward Rate Constants

The forward rate equation used by the program is:

$$k_f = A_f T^{P_f} \exp(E_f/RT)$$

where T is temperature in degrees Kelvin and R = 1.98725 (cal/mol-°K), P = dimensionless constant, E = (cal/mol), and A should be units such that k_f is in units of sec and moles/cm^3. Forward and backward rate constants must be input and must immediately follow the data stream that defines the chemical equation. Forward rate constants are input by using:

$KF = A_f, P_f, E_f

Examples:

(1) For a given equation $A_f = .6776 \times 10^{22}$, $P_f = -2$, and $E_f = -.10216 \times 10^6$, the input is:

$KF = .6776E22, -2, -.10216E+6

(2) For the special cases in which temperature is constant and the forward rate, therefore, is constant, only an A_f need be input.

Thus, if $k_f = 10^9$, write

$KF = 1.E+9

c. Reverse Rate Constants

The rules that apply to the forward rate constants also apply to the reverse rate constants.

Example:

If the reverse rate equation is $k_b = .2 \times 10^{20} T^{-1} \exp(0/RT)$, write

$KB = .2E20, -1., 0.

d. Catalytic Species

This data stream specifies the species making up the catalyst together with their weighting factors. The key word is MI, where I is an integer indicating this is the Ith catalytic species being input. The parameter field consists of sets each comprising a weighting factor (a number) followed by a species.

Example:

$M5 = .5H, AR, 1.5F

defines the fifth catalyst set; the missing weighting factor for argon is assumed equal to unity. Note that $M4 = * defines the fourth catalyst set to include all the species present in the system.

e. Global Catalyst Set

A global catalyst G_r is defined by

$$G_r = \frac{\prod_j X_j^{a_{r_j}}}{B_r \prod_j X_j^{b_{r_j}} + C_r}$$

where a_{r_j}, b_{r_j}, B_r, and C_r are input constants and X_j = mol/cm^3 of species j. The general format for this data stream is

$GR = B_r, C_r, species$_1$, a_{r_1}, b_{r_1}

species$_2$, a_{r_2}, b_{r_2}, ..., species$_j$, a_{r_j}, b_{r_j}

where r is an integer indicating this is the rth global catalyst. If $C_r = 0$ on input, it is assumed the entire denominator equals unity [see example (2) following].

Examples:

(1) $G1 = 1.7E14, 3.24E-3, CL2 = 1.5, 0, CL = 0, 2

implies

$$G1 = \frac{(Cl_2)^{1.5}\ (Cl)^0}{1.7E14(Cl_2)^0\ (Cl)^2 + 3.24E\text{-}3}$$

(2) $G2 = 1, 0, CL = 1.7, 0

implies

$$G2 = (Cl)^{1.7}$$

f. Rate Constants Temperatures

Three temperatures, T_1, T_2, and T_3, to be used in the computation of either the forward or backward rate constant that has not been input, are specified by:

$T RATES = T_1, T_2, T_3

If this option is not used, the program sets T_1 = 298 K, T_2 = 3000 K, and T_3 = 6000 K. The computation is performed using the equation $k_f/k_b = K$ where K is the equilibrium constant.

Example:

If T_1 = 5400, T_2 = 5690, and T_3 = 5900, then

$T RATES = 5400, 5690, 5900

7. INTEGRATION CONTROLS

a. Integration Step Size Control

The user can control the initial step size to be used in one of two ways.

(1) δT

Under this option, the step size = $\delta T/|dT/dx|$. The quantity in the denominator is the absolute value of the temperature derivative at the starting x. The program uses this step size for the first five steps.

(2) Δx, N

Under this option, both the initial step size Δx and N, the number of steps Δx that is to be used, are input.

If this data stream is not used, the program sets δT = 3 and chooses the initial step size according to (1). The formats for this data stream are:

$STEP = δT

$STEP = Δx, N

If two numbers are input in the STEP parameter field it is assumed that option (2) is being used.

Examples:

(1) $STEP = 1

indicates $\delta T = 1.$

(2) $STEP = 2.5E-8, 2

indicates Δx = 2.5E-8 and N = 2

b. Integration Method and Controls

This data stream controls the choice of integration methods. If this stream is not present, the program assumes that the Runge Kutta method is to be used and the initial step size is determined by the $STEP function. The data stream for the Holt-Gear technique is as follows

$INTEG = HOLT, ERROR = number, HMIN = number, HMAX = number,
NPRNT = number, YMIN = number, EPSN = number

where ERROR is the relative accuracy desired; the recommended range is 1.E-6 $\leq$ ERROR $\leq$ 1.E-4. HMIN is the minimum step size and HMAX is the maximum step size. NPRNT is an optional print control such that NPRNT =

0	no extra print
1	print x, h, $y_i(x)$, $y_i'(x)$
2	print the above plus $y_i(x)$ predicted
3	print the above plus BND*YMAX(1), ICONV(I)
4	print the above during the Newton iteration

YMIN is an estimate of absolute zero, $y_i(x)$ min, used in the relative error test.

Tests for a specific problem have been adequately solved with the use of EPSN = 1.E-13; however, the user can experiment for specific problems with the use of smaller or larger values for EPSN. If EPSN > 1.E-10, it is set to 1.E-13.

Example:

$INTEG, HOLT, ERROR = 1.E-4, HMIN = 1.E-15,
HMAX = 20, YMIN = 1.E-11, EPSN = 1.E-13, NPRNT = 0

The data stream for the Emanuel-Aitken method is $INTEG = EMANUEL, Q1 = number, HMAX = number, HMIN = number, DEFAULT = number, RATIO = number, WOBBLE = number, DOUBLE = number, where Q1 is an integer such that if the integrated value for the moles per gram of any species greater than 10^{Q1}, an absolute error test is used for that species. This effectively prevents species in small concentrations from governing the step size. HMAX and HMIN are the maximum and minimum allowable step sizes, respectively. The error is kept between a value equal to DEFAULT and DEFAULT/RATIO. The variance in the estimate of the derivatives is kept less than a value equal to WOBBLE, and the doubling criterion must be passed DOUBLE steps before the step size is increased.

Keywords DEFAULT, RATIO, WOBBLE, and DOUBLE need not be specified. The program default values are shown on the example card.

Example:

$INTEG = EMANUEL, Q1 = -8, HMAX = 2, HMIN = 1.E-4, DEFAULT = 1.E-4, RATIO = 20, WOBBLE = .03, DOUBLE = 2

8. CONTOURS

For each of the five contours described in the following paragraphs, a set of coordinates describing the contours is input. A maximum of 100 coordinates can be input. If only one point is input, the contour is assumed constant. If two points are input, the program interpolates linearly to find intermediate results. Quadratic interpolation is used when more than two points are input.

a. Area Contour

When this data stream is used, it is assumed that the flow is a rocket or wind tunnel nozzle or an expanding flow type. The area contour (in square centimeters) is input as:

$AREA VS X = A_1, x_1, A_2, x_2,....

where A_i is the contour area at distance x_i. (x_i is the time if the quiescent gas option is on.)

Example:

$AREA VS X = 1, 0, 5.4, 1, 45, 10 specifies area values 1, 5.4, and 45 at distances 0, 1, and 10.

b. Radius Contour

This option can be used instead of the area contour whenever it is more convenient to input the radius contour. The radius contour (in centimeters) is input as:

$RADIUS VS X = r_1, x_1, r_2, x_2,...

where r_1 is the value of the radius at distance x_i.

c. Pressure Contour

When this data stream is used, it is assumed that the flow type is a pressure streamtube (P STREAM). The pressure contour (in standard atmospheres) is input as:

$P VS X = p_1, x_1, p_2, x_2,...

where p_1 is the system pressure at distance x_1. (x_1 is time if the quiescent gas option is on.)

Example:

$P VS X = .38, 0, .32, 4.E-4, .11, 7.E-3 specifies pressures of 0.38, 0.32, and 0.11 atm at x = 0, 4.E-4, and 7.E-3, respectively.

d. Density Contour

When this data stream is used, it is assumed that the flow type is a density streamtube (RHO STREAM). The density contour (grams per cubic centimeter) is input as:

$RHO VS X = ρ_1, x_1, ρ_2, x_2, ...

where ρ_i is the system density at distance (time) x_i.

Example:

$RHO VS X = 1.09E-5, 0, 1.08E-5, 10

specifies densities 1.09E-5 and 1.08E-5 at points 0 and 10, respectively.

e. Temperature Contour

When this data stream is used, it is assumed that the flow type is a temperature streamtube (T STREAM). The temperature contour (in degrees Kelvin) is input as:

$T VS X = T_1, x_1, T_2, x_2 ...

where T_i is the temperature at distance (time) x_i.

Example:

$T VS X = 3000, 0 indicates the temperature is 3000 K at x = 0, and since only one temperature point is input, the temperature is assumed to be constant.

9. FLASHLAMP OPTIONS

a. Photodissociation Reactions

Equation IIB-15 of Ref. 1 was modified as follows:

$$\left(\frac{dn_i}{dt}\right)_{ph} = \frac{c_i Z_{i[I(t)]}}{\rho} \left\{1 - \exp\left[-Z_2 \rho \left(\frac{n_a}{g_a} - \frac{n_b}{g_b}\right)\right]\right\}$$

This change was made to permit more accurate modeling of conditions wherein a species in an excited state is formed, rather than dissociation products. Default values of $g_a = g_b = 1$ and $n_b = 0$ are built into the program.

A maximum of five photodissociation reactions can be input. The format of the photodissociation reactions data stream is $FLASH, ABSORB, Z1 = number, Z2 = number, VA = number, GA = number, GB = number, NB = species name, species name = c_1, species name = c_2, ABSORB, etc. The order following ABSORB may vary.

ABSORB = label indicating the start of a parameter string containing constants for one reaction

Z1 = maximum number of moles of laser gas available in moles per second per cubic centimeter

Z2 = laser gas absorption parameter in cubic centimeters per mole

VA = photon frequency in sec^{-1}

GA = degeneracy of the state, $c_i = -1$ (dimensionless).

GB = degeneracy of the state, $c_i = +1$ (dimensionless). Default value = 1.

NB = name of species produced by absorption. Default value = 0.

The sets of pairs of species $name_i = c_i$ contain the name of a species and its value of c_i where c_i is:

-1 if the species is dissociated by photons

+1 if the species is produced by photons

+2 if 2 molecules of species i are produced by dissociating one molecule

(For all other species, no c_i is input.)

Example:

This example illustrates the input for a case in which only one reaction is needed; F_2O is the absorbing species and no species b is needed.

```
$FLASH, ABSORB, Z1 = .129, Z2 = 2.3E5,
VA = 1.55E15, F = 1, F0 = 1, F20 = -1
```

This example illustrates a case in which only one reaction is needed, HBR/79/(4) is the absorbing species.

```
$FLASH, ABSORB, Z1 = .15, Z2 = 2.29E6, VA = 7.4E8,
HBR/79/(4) = -1, HBR/79/(13) = +1, NB = HBR/79/(13),
GA = 1, GB = .778
```

b. Flashlamp Output Function

A table of the normalized dimensionless flashlamp output (I) as a function of time (t) must be input for each photodissociation reaction input in the FLASH data stream. A maximum of 100 points can be input in each table as follows:

$$\$I \text{ VS } T = I_1, t_1, I_2, t_2, \ldots$$

For example, if two photodissociation reactions are input, then two separate output tables must be input in the same order that the reactions appear on the $FLASH data stream.

$I VS T = 0, 0, .2, 2.5E-6, .4, .5E-6, .6, 7.5E-6, .78, 1.E-5, .9, 1.2E-5

$I VS T = 0, 0, .3, = 3.0E-6, .5 6.2E-6, .6, 7.6E-6, .8, 1.1E-5, .1, 1.3E-5

The information in the following two sets of tables is implied.

$I^{(1)}$	$t^{(1)}$	$I^{(2)}$	$t^{(2)}$
0	0	0	0
.2	2.5E-6	.3	3.0E-6
.4	5.0E-6	.5	6.2E-6
.6	7.5E-6	.6	7.6E-6
.78	1.0E-5	.8	1.1E-5
.9	1.2E-5	1.	1.3E-5

10. OUTPUT OPTIONS

a. Printed Output Controls

This data stream contains print control options and is of the form

$PRINT = THERM, RATES, SUMMARY, INTERVAL = number, MAX ANSWERS = number, X STOP = number, THROAT

The order in which these options appear can vary.

THERM

If this label is present, it causes a printout of the thermodynamic data library tables for each species in the system.

RATES

If this label is present, the values of KF, KB, LF, LB, and (LF - LB) are printed at each answer station.

SUMMARY

If this label is present, the engineering summary tables are printed for rocket and wind tunnel performance only.

INTERVAL = number

This label specifies the integration step where answers are to be printed.

INTERVAL = 1 causes printout at the end of each integration step.

MAX ANSWERS = number

This label specifies the maximum number of answer sets to be printed.

X STOP = number

This indicates the last answer station, i.e., value of the independent variable (distance or time).

THROAT

This label can be used for rocket and wind tunnel runs for answer printout at the chamber and throat locations only.

Example:

$PRINT, MAX ANSWERS = 100, INTERVAL = 20, RATES, X STOP = 45

b. Plot Output Control

Plots can be obtained for the flow types listed in Table 3. The keyword PLOT is followed by the list of variables to be plotted. The individual variables must be separated by either a comma or a slash, a comma indicates that the next variable is to be plotted on the same set of axes as the preceding variable (a maximum of nine variables can be plotted on a single set of axes), and a slash indicates that the following variable is to be plotted on a new set of axes.

The designations used to identify the variables are derived from the printed output. The basic designations recognized by the program are shown in Table 10.

Table 10. Basic Designations

Plot Designation	Variable
P	Pressure
T	Temperature
H	Enthalpy
S	Entropy
R	Density
W	Weight flow
CP	Specific heat at constant pressure
G	Ratio of specific heats
M	Mach number
V	Flow velocity
AREA	Flow area
SIGMA[1]	
GAM1[1]	
GAM2[1]	
LAMBDA1[1]	
LAMBDA2	
A	Acoustic velocity
I	Normalized flashlamp output function

[1]Defined in Ref. 1.

The molar concentration of a species is designated by the name of the species, which must be identical to the name as it appears on the thermodynamic data tape. An alternative designation is "CONC(S_1, S_2,...)" where the S_1, S_2, etc., are species names. The latter form must be used for the species H, S, and I to avoid confusion between these species and the designations for enthalpy, entropy, and the normalized flashlamp output function.

Partial derivatives can also be plotted; their proper designations are listed in Table 11.

Note that the partials for temperature, area, density, and pressure can be combined, e.g., D(R,T)/DX will cause the partial derivatives of both density and temperature to be plotted.

To plot the rate of production of a chemical species, the name of the species is inserted within the parentheses of the designation D( )/DX. For flashlamp cases, D( )/DX or CHEM D( )/DX designates photon rates of production. More than one species name can be included within the parentheses.

To plot rate equation data, the appropriate designation is used with the desired equation numbers inserted within the parentheses. The designations recognized by the program are listed in Table 12.

Example:

$PLOT, KF(3,10/1), LF(5)/H, S/H2, CONC(H)/D(HF(0), FO)/DX/AREA
will produce six separate plots, as follows:

Plot number	Contents
1	KF rate data for equations 3 and 10
2	KF rate data for equation 1 and LF rate data for equation 5
3	Enthalpy and entropy
4	Molar concentrations for H_2 and H
5	Rates of production for HF(0) and FO
6	Flow area

Table 11. Derivative Designations

Plot Designation	Variable
D(T)/DX	Partial derivative of temperature
D(A)/DX	Partial derivative of area
D(R)/DX	Partial derivative of density
D(P)/DX	Partial derivative of pressure
DX	Step size
DTIME	Step size for quiescent gas

Table 12. Rate Equation Designations

Plot Designation	Variable
KF( )	Forward rate constant
KB( )	Backward rate constant
LF( )	Rate of reaction in forward direction
LB( )	Rate of reaction in backward direction
LF( ) - LB( )	Net reaction rate, i.e., rate of reaction in forward direction minus rate in backward direction.

Notes

a. The maximum number of items that can be plotted is 100

b. If $SETGRID is not used, the plot program automatically selects the grid and scaling. If more than one item is to be plotted on the same set of axes, the grid and scaling will be selected on the basis of the first item only.

c. All data points used in the plots are automatically taken from the normal program output.

d. Excited species are permitted. The species names are employed in the same manner as unexcited species names.

e. The program will not interpret the slash mark that appears as a part of the partial derivative and rate of production designations as signifying that a new plot will be started.

f. No comma or slash should be placed after the last item.

g. All variables are plotted as a function of particle time.

c. Plot Grid and Scaling Controls

This data stream can be used to override the automatic scaling of axis and the choice of grid by the NEST plot program. The keyword SETGRID is followed by the frame number, the grid type, and scaling information as follows:

$SETGRID, FRAME = 1, GRID = XXX, XMIN = value, XMAX = value, XDELTA = value, YMIN = value, YDELTA = value, YSCALE = value, FRAME = 2, GRID = ...

The GRID patterns that can be used are listed in Table 13.

XMIN = starting point for X axis of plot. Any value less than XMIN will be discarded.

XMAX = maximum value along the X axis. Any value greater than this will be discarded.

XDELTA = number of units per inch along the X axis. If optimum scaling along the X axis is desired, then appropriate values for XDELTA are -1 for 10-in. plots, -2 for 20-in. plots, -3 for 30-in. plots, and -4 for 80-in. plots

YMIN = lowest or starting point for the Y axis.

YDELTA = number of units per inch along the Y axis.

YSCALE = for log plots only, minus the number of inches per cycle. See Table 13 and use YDELTA = 0.

Table 13. Plot Grid Selection

Type	Grid Number	Description
No grid	300	
Square grids	301	X 10 divisions per inch Y 10 divisions per inch
	302	X 20 divisions per inch Y 20 divisions per inch
	3A1	1-in. border on left X 10 divisions per inch Y 10 divisions per inch
	3A2	1-in. border on left X 20 divisions per inch Y 20 divisions per inch
	3B1	1-in. border on left and right X 10 divisions per inch Y 10 divisions per inch
	3B2	1-in. border on left and right X 20 divisions per inch Y 20 divisions per inch
	3CM	1-in. border on left, 0.25-in. border on right (grid size 17 × 9.84 in.) X 10 divisions per 0.79 in. (5 divisions per centimeter) Y 10 divisions per 0.79 in. (5 divisions per centimeter)
Rectangular grids	3AS	1-in. border on left, 0.7-in. border on right X 5 divisions per 0.85 in. Y 10 divisions per inch
	3BS	1-in. border on left X 10 divisions per 0.8 in. Y 10 divisions per inch
Semi-log grids	3AL	1-in. border on left and right X 10 divisions per 0.6 in. Y 4 cycles, 2.5 in. per cycle

Table 13. Plot Grid Selection (con't.)

	3BL	1-in. border on left (grid size 17 × 9.8 in.) X 10 divisions per inch Y 7 cycles, 1.4 in. per cycle
	3DL	1-in. border on left and right X 10 divisions per inch Y 5 cycles, 2 in. per cycle
	3KL	1-in. border on left X 20 divisions per inch Y 3 cycles, 3.33 in. per cycle
	3ML	1-in. border on left X 20 divisions per inch Y 8 cycles, 1.25 in. per cycle
	3NL	1-in. border on left and right X 2 cycles, 7.5 in. per cycle Y 10 divisions per inch
	3OL	1-in. border on left and right X 3 cycles, 5 in. per cycle Y 10 divisions per inch
	3PL	1-in. border on left X 20 divisions per inch Y 5 cycles, 2 in. per cycle
Log-log grids	3CL	1-in. border on left and right X 2 cycles, 7.5 in. per cycle Y 2 cycles, 5 in. per cycle
	3EL	1-in. border on left X 8 cycles, 2 in. per cycle Y 5 cycles, 2 in. per cycle
	3FL	2-in. border on left, 1-in. border on right X 7 cycles, 2 in. per cycle Y 5 cycles, 2 in. per cycle
	3GL	1-in. border on left and right X 5 cycles, 3 in. per cycle Y 5 cycles, 2 in. per cycle

Table 13. Plot Grid Selection (con't.)

3HL	2-in. border on left X 5 cycles, 3 in. per cycle Y 5 cycles, 2 in. per cycle
3JL	1-in. border on left and right X 2 cycles, 7.5 in. per cycle Y 5 cycles, 2 in. per cycle

Example:

$SETGRID, FRAME = 1, GRID = 3BL, XDELTA = -1,
YMIN = 1.E-14, YDELTA = 0, YSCALE = -1.4, FRAME = 2

implies two plots are to be made with automatic X axis scaling on 7-cycle semi-log paper with a minimum of 1×10^{-14} for the Y axis.

Dimensions for all grids, including margins, are 17 in. (x) by 10 in. (y), except where otherwise noted, with 5/8 reduction for CDC HARDCPY.

d. Program Trace

The program trace flag, ID3R, can be set by the following:

a. $DUMP = ON
   sets ID3R = -1

b. $DUMP = OFF
   sets ID3R = 0

c. $DUMP = ON, N
   sets ID3R = N

e. Observer Velocity

The velocity relative to the observer (in centimeters per second) is used to compute and print particle time for Table 3 flow types. The input format is

$V OBSERVER = number

Example: $V OBSERVER = 25000

11. SPECIAL PROGRAM CONTROLS

a. Program Flags

This option permits the user to alter some of the built-in flags in the program. Table 14 contains a list of these flags, which are input as follows:

$FLAGS, $f_1 = n_1$,$f_2 = n_2$,...

f_1, f_2, are flag numbers that are to be set to n_1, n_2, etc.

Table 14. Special Option Flags

Flag	Description
2	Starting temperature for flame solution if different from 3000 K.
11	Rocket exit area (cm^2).
12	Value of inlet area for nonequilibrium runs (not including rocket and wind tunnel); default value is 1 cm^2.
13	Internal energy computed from input conditions is increased by an amount equal to the value of flag 13 before the constant volume combustion calculation is performed.
14	If flag 14 is nonzero, the L_{fr} and L_{br} arrays are computed based on the equilibrium chamber conditions in the rocket overlay. These values are printed and the program immediately returns to the input overlay.
15	Stability parameter B, set = 1 unless flag 15 is used.
17	If flag 17 is nonzero, extra printout is provided during the calculation, in the input overlay, of the state variables not specified on input cards.
18	Value of the mass flow in rocket and wind tunnel cases. Alternative use: if ≠0, return to the input overlay for the next case after detecting errors in ESHOCK (otherwise exit).
19	Contains the throat area (cm^2) for rocket and wind tunnel cases. Alternative use: if ≠0, punch concentrations of excited species in laser constant density runs.
20	≠0, print L_{fr} and L_{br} arrays at every step during the ROCKET overlay equilibrium computations.
29	Normally = 100; if the max/min ratio of a variable to be plotted is greater than the input value of flag 29, use log plots.
30	If the system freezes in ESHOCK, i.e., if the percent temperature difference between corresponding frozen and equilibrium solutions is less than flag 30, then compute only the frozen conditions for the remaining velocities.
31	The computation is terminated in SHOCK when the Mach number is less than flag 31.

32	In the rocket and wind tunnel summary table, flag 32 (normal value = 1) is the amount the area ratio is incremented to print the next set of answers.
34	Any area downstream of the throat (set equal to 3 normally). See flag 35.
35	Number of print stations to be used between the throat and the area of flag 34 (set equal to 32 normally).
37	≠0, for a concise trace printout in ROCKET and NEQUIL.
38	If nonzero, flag 38 equals the x coordinate at which the card type 10 answer interval is to be overridden and printing begun of answers at every step in overlays SHOCK and CALC.
39	In SHOCK and CALC, flag 39 equals the x coordinate at which the dump flag ID3R is to be set equal to -1. In ESHOCK, flag 39 equals the decimal number R.C, where R represents the run number and C the case number at which the dump flag ID3R is set equal to -1.
40	If δ (divergence point parameter) is less than flag 40, departure from equilibrium has occurred in ROCKET. (Flag 40 is normally set equal to 0.015).
42	Flag 42 equals the maximum allowable integration step size (normally set equal to 0.2 cm).
49	Maximum number of NEST printout pages permitted.

Example:

$FLAGS, 42 = 5

sets the maximum allowable integration step size, i.e., flag 42 equal to 0.5 cm.

12. EDIT CONTROLS

a. End of Case

Each case must end with $END.

b. New Case

The new case data stream is

$NEW CASE

All complete new cases, with the exception of the first case, must begin with this data stream.

c. Multiple Case Runs

Multiple case runs can be handled by the input program. The run may consist of the stacking of complete cases, the updating of previously input cases, or both; however, the deck setup and assumptions differ for the two situations.

(1) Complete Case Stacking

A complete case consists of all the necessary input data for the solution of one set of conditions for one flow type. The method of stacking complete cases is illustrated in Fig. 1. Note that all cases but the first begin with $NEW CASE.

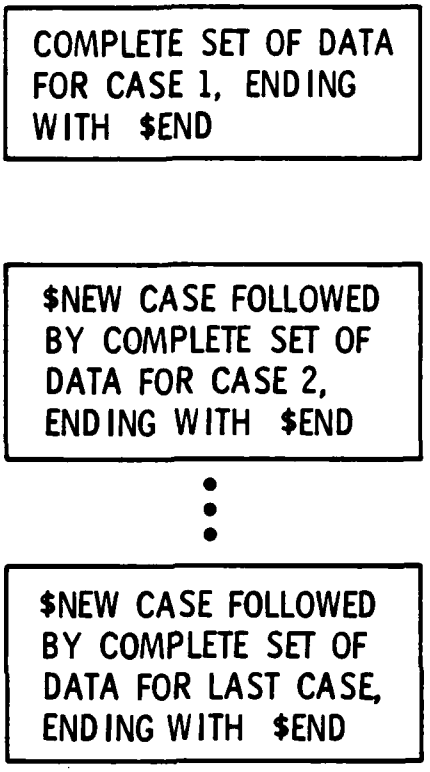


Fig. 1. Complete Case Stacking

(2) Updating of Cases

In this situation, the complete set of data for the first case (terminated by $END) is followed by sets of items (each set terminated by $END) to be updated in the previous case. The quantities that can be updated are restricted; the following data streams cannot be repeated after the first case is input.

a. $FLOW
b. $ATOMS
c. $QATOMS
d. $EXCITE
e. $INCL
f. $EXCL
g. $HEAT
h. $JANAF DATA
i. $EQ
j. $M
k. $G

The major items in the system, i.e., atomic composition, flow type, system species, and reaction equations, therefore, cannot be updated. In Fig. 2 the method of using the update feature is illustrated. The first complete case is input, terminated by $END, and followed by a set of data updating the first case.

In the second case to be executed, the title, system temperature, and forward rate for the reaction with serial number 15 are updated.

```
$TITLE = CASE 1
$ATOMS = H, F, AR
$FLOW = RHO STREAM, $T = 5000
  -
  -
$EQ 15, 2H = H2  $KF = 5E19, -1, 0
  -
  -
  -
$END
```

```
$TITLE = CASE 2
$ T = 4000, $KF15 = 5.4 E 19, -1, 0
$END
```

•
•
•

```
$TITLE = LAST CASE
$ T = 2300, $KF 15 = 4.12 E 19, -1, 0
$END
```

Fig. 2. Updated Case Run

III. CONTROL CARDS

The following control cards must be used to run the NEST Program.

```
ATTACH, TAPE5, 8TAPE5, ID = 09680.
ATTACH, MAIN, 4NESTMAIN, ID = 06629.
ATTACH, L, 4NESTSUBS, ID = 06629.
ATTACH, PLOTLB, 3FTNPLOTLB.
LDSET, LIB = L/PLOTLB, PRESET = ZERO, MAP = 0.
MAIN.
```

IV. SAMPLE INPUT SHEETS

Seven sample cases are presented in this section. These cases were prepared for demonstration purposes only; it should not be assumed that any quantities such as rate constants or heats of formation are accurate.

The first sample input sheet is a typical nonequilibrium problem. The flow type, specified on the second card, is a constant pressure case. Since the composition is input in mol/cm^3 and the temperature is specified on card 3, the program can compute the pressure of the system. This pressure information completes the program requirement that two state variables be input, and since the pressure is not specified in the input, it is assumed that this is a constant pressure problem. The $INTEG data stream was omitted, so the default Runge-Kutta integration method will be used with the initial δT specified on the $STEP data stream. Card 5 sets the output controls for printout at every second integration step; the problem is completed when either the variable X exceeds 10 cm (i.e., XSTOP) or a maximum of 100 answers is printed.

```
CARD NO.     1      $TITLE=PRESSURE STREAMTUBE
CARD NO.     2      $ATOMS=C,O,H,N    $FLOW=P STREAM
CARD NO.     3      $T=518    $VEL=2.92531E5
CARD NO.     4      $STEP=.0005
CARD NO.     5      $PRINT,INTERVAL=2,MAX ANSWERS=100,XSTOP=10
CARD NO.     6      $MOL/CC,CO2=.53+7E-9,H2=.1933E-9,H=.1145E-10,
CARD NO.     7      H2O=.9J6E-9,OH=.67E-1.,O=.2877E-12,CO=.6045E-9
CARD NO.     8      $PLOT,T/CONC(H,O,OH,H2O,HO2)/CO,CO2,H2,N2,O2
CARD NO.     9      $SETGRID,FRAME=1,GRID=302,XMIN=0,XMAX=.02,
CARD NO.    10      XDELTA=.0.2,YMIN=500,YDELTA=5,FRAME=2,GRID=33L,
CARD NO.    11      YMIN=1.E-14,YDELTA=3,YSCALE=-1.+,FRAME=3
CARD NO.    12      $M1=H,N,O,HO,H2O,H2,CO,CO2,NO,N2,O2
CARD NO.    13      $EQ=CO2,+M1=CO,+O,+M1          $KB=.1E17,0,-3500.
CARD NO.    14      $EQ=H2O,+M1=OH,+O,+M1          $KB=.1E20,-1.
CARD NO.    15      $EQ=H2,+M1=2H,+M1              $KB=.75E19,-1.
CARD NO.    16      $EQ=CO2,+H=CO,+OH              $KB=3.1E11,0,-6000.
CARD NO.    17      $EQ=H2O,+H=OH,+H2              $KB=.6E12,.5,-5000.
CARD NO.    18      $EQ=HO2,+H=H2,+O2              $KF=1.E11,.5,-6000.
CARD NO.    19      $EQ=O2,+H2=2OH                 $KF=.1E15,0,-.75E5
CARD NO.    20      $EQ=N2,+O2=2NO                 $KF=.2E15,0,-.122E6
CARD NO.    21      $EQ=CO,+O2=O,+CO2              $KF=.35E13,0,-.51E5
CARD NO.    22      $END
```

All eight cases described in Table 4 are to be calculated. Either the system pressure or density must be input and the ambient temperature must be specified; in this case T = 299.2 K. The eight cases are to be calculated for each input velocity.

```
CARD NO.    1    $TITLE=EQUILIBRIUM/FROZEN SHOCKTUBE
CARD NO.    2    $FLOW=INCIDENT,REFLECTED    $ATOMS=H,O,AR
CARD NO.    3    $P=.665789-7,ATM   $T=299.2
CARD NO.    4    $MOL PCT,H2O=1,AR=99
CARD NO.    5    $VEL=1.-8,1.-4      $END
```

This is an equilibrium rocket performance problem and is so specified on card 2. The system pressure must be input for a rocket case. The heats of formation, used to calculate the system enthalpy, are input for the components that appear on the CHAMBER card. Card 5 contains a very complex chemical name for one of the system species, $C_{.117}H_{9.5855}O_{1.684}N_{.1384}$. This is the only data stream where fractional subscripts may appear in the species name. Card 3 sets flag 11, the nozzle exit area, equal to 50.

```
CARD NO.    1    $TITLE=EQUILIBRIUM ROCKET PERFORMANCE
CARD NO.    2    $ATOMS=AL,H,N,CL,O,C      $FLOW=ROCKET,EQ
CARD NO.    3    $P=46,MM   $FLAGS,11=50       $PRINT,SUMMARY
CARD NO.    4    $CHAMBER,CHEM=AL,HEAT=0,WT PCT=17,
CARD NO.    5    CHEM=H4NCLO4,HEAT=-70.73,WT PCT=65,
CARD NO.    6    CHEM=C.117H9.5855O1.684N.1384,HEAT=-82.8,WT PCT=18
CARD NO.    7    $END
```

This input sample is a wind tunnel problem for the calculation of equilibrium conditions and then the calculation of the nonequilibrium chemistry after departure from equilibrium. The flow type is defined on card 2. The $M, $EQ, and $KF data streams are for use in the nonequilibrium calculation. The nozzle shape is defined by the $AREA VS X data stream starting on card 15. The $PRINT data stream is for output during the nonequilibrium calculation; the equilibrium portion will automatically print answers at 48 stations.

```
CARD NO.    1    $TITLE=WINDTUNNEL, EQUILIBRIUM AND NON EQUILIBRIUM
CARD NO.    2    $FLOW=WIND,EQ,NONEQ    $ATOMS=O,N
CARD NO.    3    $P=1200,ATM    $T=7360
CARD NO.    4    $MOL/GM,O2=.5393356?E-3,N2=.2415030 4E-1,NO=.3940631 1E-2,
CARD NO.    5              N=.2519801 5E-2,O=.9537491E-2
CARD NO.    6    $M1=O2    $M2=O      $M3=N,N2,NO    $M4=*
CARD NO.    7    $EQ=O2, + M1 = 2O, + M1          $KF=.1112E26,-2.5,-.117204E6
CARD NO.    8    $EQ=O2, + M2 = 2O, + M2          $KF=.1112E26,-2.5,-.117204E6
CARD NO.    9    $EQ=O2, + M3 = 2O, + M3          $KF=.1112E26,-2.5,-.117204E6
CARD NO.   10    $EQ=N2, + M4 = 2N, + M4          $KF=.7838E26,-2.5,-.224475E6
CARD NO.   11    $EQ=NO, + M4 = N, + O, + M4      $KF=.2296E26,-2.5,-.148988E6
CARD NO.   12    $EQ=O, + N2 = N, + NO            $KF=1.E12,.5,-75487.
CARD NO.   13    $EQ=O2, + N = O, + NO            $KF=.1014E12,.5,-6198.
CARD NO.   14    $EQ=O2, + N2 = 2NO               $KF=.2699E14,0,-.106874E6
CARD NO.   15    $AREA VS X, .73516,0, .45876,.5, .26517,1, .12438,1.5,
CARD NO.   16    .11442,1.5494, .11852,1.651, .14872,2, .20068,2.5, .26202,3,
CARD NO.   17    .56312,5, .98224,7, 1.87464,10
CARD NO.   18    $PRINT,INTERVAL=20,MAX ANSWERS=200,XSTOP=10    $END
```

The purpose of this equilibrium rocket performance calculation is to calculate the area at the nozzle throat. The temperature, pressure, and cold pressure must be input. In addition, the mass flow and heat of formation of each system component must be input by means of the $CHAMBER data stream.

It is often of interest to run the reverse of this case, that is, to input the throat area and total mass flow of the system so that the program can calculate the chamber temperature. If the total mass flow and area are specified by means of flags 18 and 19. respectively, it is assumed that the chamber temperature is to be calculaced.

```
CARD NO.    1     $TITLE=ROCKET NOZZLE THROAT AREA CALCULATION
CARD NO.    2     $FLOW=ROCKET,EQ   $ATOMS=HE,S,F,O
CARD NO.    3     $T=2[illegible]   $P=64[illegible],PSIA,$OLD=329     $POINT,THROAT
CARD NO.    4     $CHAMBER,CHEM=HE,MASS FLOW=2.2,HEAT=0,
CARD NO.    5     CHEM=SF6,MASS FLOW=2.7,HEAT=-291.7,
CARD NO.    6     CHEM=O2,MASS FLOW=.57,HEAT=0
CARD NO.    7     $END
```

The input for the General Solver case and the Mollier case presented here are very similar. The General Solver case uses the $INCL data stream to limit the total number of species in the system to the five species listed in this data stream. If the $INCL is not present, all species on thermodynamic tape comprised of N and O atoms would be included in the system.

In the Mollier solution case, a fuel and an oxidizer are present with a mixture ratio of 28.7. Note that the label FUEL is included after the methane is defined so that the program can identify which of the two species is the fuel.

```
CARD NO.    1    $TITLE=GENERAL SOLVER
CARD NO.    2    $ATOMS=N,O      $FLOW=GEN SOLVER
CARD NO.    3    $T RANGE=6000,4000,250    $P RANGE=1200,1200,0
CARD NO.    4    $INCL=N,O,N2,O2,NO
CARD NO.    5    $MOL/GM,O2=.53933557E-3,N2=.24150304E-1,
CARD NO.    6    NO=.39436311E-2,N=.25198005E-2,O=.95374 1E-2
CARD NO.    7    $END
```

```
CARD NO.    1    $TITLE=MOLLIER SAMPLE CASE    $ATOMS=C,H,N,O
CARD NO.    2    $FLOW=MOLLIER    ET RANGE=2020,1500,20
CARD NO.    3    $PRANGE=10,9,1
CARD NO.    4    $CHAMBER,CHEM=CH4,,LABEL=METHANE,FUEL,MIX=28.7,
CARD NO.    5    CHEM=0.4205N1.58,LABEL=AIR    $END
```

APPENDIX

NEST EXPANDED VERSION - AEROSPACE ONLY

This version of NEST was developed for the running of nonequilibrium cases involving large number reactions and species.

RESTRICTIONS

1. 2000 total number of reactions
2. 125 species
3. 15 elements
4. 20 catalyst sets with ≤ 100 species per set
5. One global catalyst
6. 16 flash lamp functions
7. A species may appear in at most 250 chemical reactions
8. 8 analytic flash lamp functions are available

ADDITIONAL SPECIAL OPTION FLAGS

16 = 1, the long printout of the forward and reverse rate constants plus the reaction species that appears before the actual NEST calculation begins will be suppressed.

33 x coordinate where rate printout is to start. (Omit RATES on $PRINT input.)

34 x coordinate where rate printout is to cease.

53 = 1, suppress the printout for the rate of production for each species at each print station.

56 = 0, vibrational species (default)
= 1, HF(v,J) v=0,6 J=0,40
= 2, DF(v,J) v=0,6 J=0,40
= 3, H_2(v,J) v=0,1 J=0,15
= 4, D_2(v,J) v=0,1 J=0,15
= 5, HD(v,J) v=0,1 J=0,15

For a calculation using more than one of the above species, i.e., HF(v,J) + H_2(v,J), $FLAG56=13

101 = Analytic flash lamp number (1-8)

102 = Input information for analytic flash lamp

.
.
.

150 =

TIMING

Note that increased running time is most dependent on the total number of species in the system and less dependent on the total number of reactions.

CONTROL CARDS

The following files must be attached if the expanded version of NEST is used

4MAINEXPAND, ID=06629

4SUBSEXPAND, ID=06629

LABORATORY OPERATIONS

The Laboratory Operations of The Aerospace Corporation is conducting experimental and theoretical investigations necessary for the evaluation and application of scientific advances to new military space systems. Versatility and flexibility have been developed to a high degree by the laboratory personnel in dealing with the many problems encountered in the nation's rapidly developing space systems. Expertise in the latest scientific developments is vital to the accomplishment of tasks related to these problems. The laboratories that contribute to this research are:

Aerophysics Laboratory: Launch vehicle and reentry aerodynamics and heat transfer, propulsion chemistry and fluid mechanics, structural mechanics, flight dynamics; high-temperature thermomechanics, gas kinetics and radiation; research in environmental chemistry and contamination; cw and pulsed chemical laser development including chemical kinetics, spectroscopy, optical resonators and beam pointing, atmospheric propagation, laser effects and countermeasures.

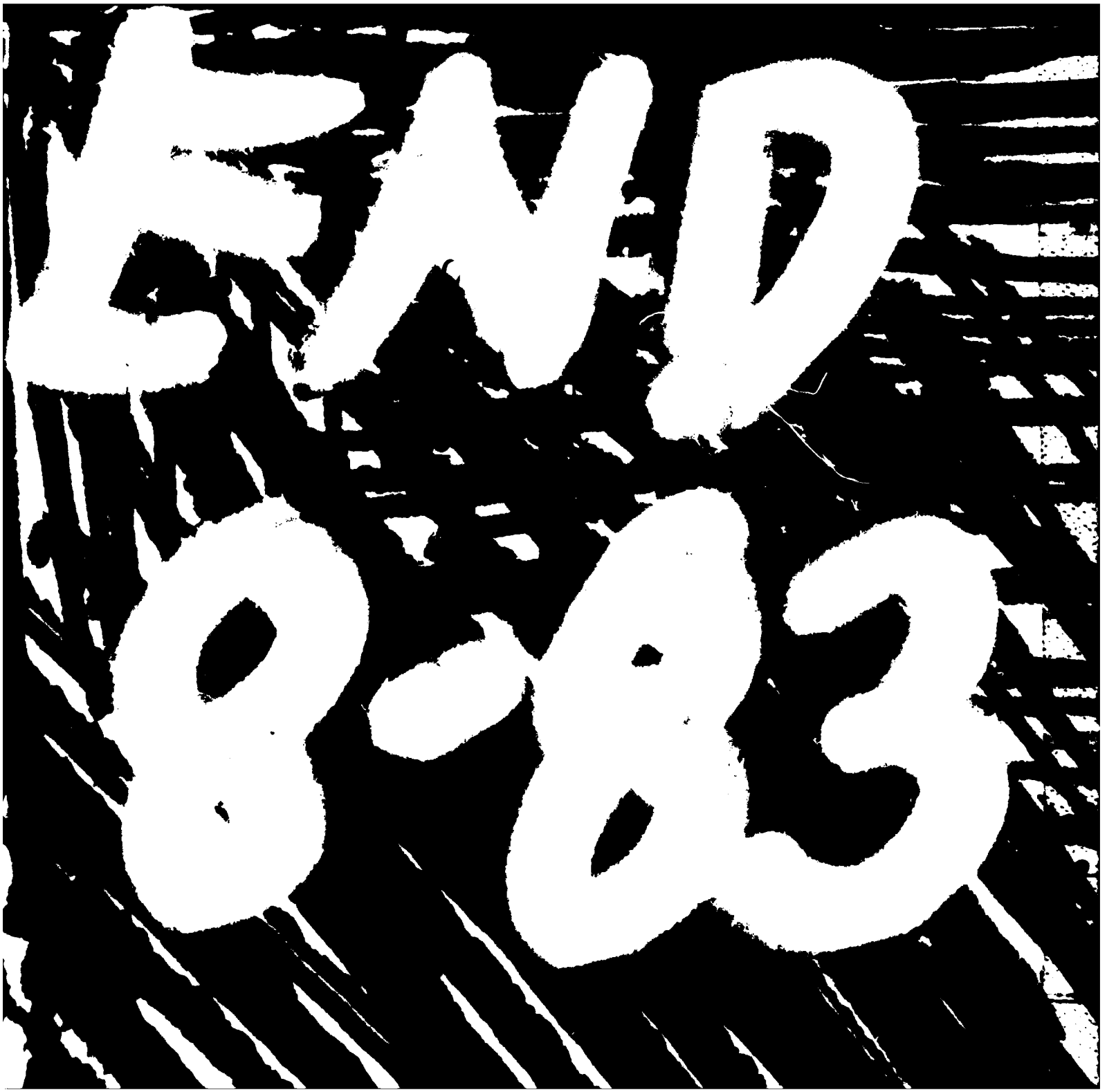
Chemistry and Physics Laboratory: Atmospheric chemical reactions, atmospheric optics, light scattering, state-specific chemical reactions and radiation transport in rocket plumes, applied laser spectroscopy, laser chemistry, battery electrochemistry, space vacuum and radiation effects on materials, lubrication and surface phenomena, thermionic emission, photosensitive materials and detectors, atomic frequency standards, and bioenvironmental research and monitoring.

Electronics Research Laboratory: Microelectronics, GaAs low-noise and power devices, semiconductor lasers, electromagnetic and optical propagation phenomena, quantum electronics, laser communications, lidar, and electro-optics; communication sciences, applied electronics, semiconductor crystal and device physics, radiometric imaging; millimeter-wave and microwave technology.

Information Sciences Research Office: Program verification, program translation, performance-sensitive system design, distributed architectures for spaceborne computers, fault-tolerant computer systems, artificial intelligence, and microelectronics applications.

Materials Sciences Laboratory: Development of new materials: metal matrix composites, polymers, and new forms of carbon; component failure analysis and reliability; fracture mechanics and stress corrosion; evaluation of materials in space environment; materials performance in space transportation systems; analysis of systems vulnerability and survivability in enemy-induced environments.

Space Sciences Laboratory: Atmospheric and ionospheric physics, radiation from the atmosphere, density and composition of the upper atmosphere, aurorae and airglow; magnetospheric physics, cosmic rays, generation and propagation of plasma waves in the magnetosphere; solar physics, infrared astronomy; the effects of nuclear explosions, magnetic storms, and solar activity on the earth's atmosphere, ionosphere, and magnetosphere; the effects of optical, electromagnetic, and particulate radiations in space on space systems.


END
OF