Title

ODE V3.2

Application Manual

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SUMMARY

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ODE V3.2 – Application Manual

This Manual contains task-oriented instructions that show you how to use the ODE module.

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1 REFERENCE DOCUMENTS

[RD1] "PLUME V3.2" – Interface files definition. P. Chèoux-Damas. Doc. MMS : S413/RT/41.97. 24/10/97

[RD2] "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performances, Incident and Reflected Shocks and Chapman Jouguet Detonations". Grodon & Mc Bride. NASA SP-273, March 1976.

2 INTRODUCTION

The ODE code provides an analytical tool to calculate the equilibrium chemical composition of the products in the combustion chamber and the nozzle for a liquid or solid-propellant rocket engine. In addition, it calculates some theoretical thermodynamic properties of the equilibrium mixture.

3 ODE DESCRIPTION

3.1 FUNCTIONAL DESCRIPTION

A very large database for ODE (JANNAF.THE), includes the thermodynamic properties of almost all chemical species that appear as combustion products of liquid and solid propellants. ODE will consider, for equilibrium composition computations, all chemical species available in the database (about 700) and consistent with the elemental composition of the propellants.

Within the context of the plume effects, the main objectives of ODE are :

according to :

- the pressure in the combustion chamber,
- the reaction enthalpy or the chamber temperature,
- the chemical nature and the proportion of fuel,
- the expansion ratio in the nozzle (exit area to throat area ratio),

compute :

- the chemical composition of the combustion gas in the chamber, at the nozzle exit,
- the thermodynamic state of the mixture at the same location (pressure, temperature, enthalpy, entropy),
- the theoretical specific thrust of the engine (for a one-dimensional isentropic expansion),
- the mass fraction of condensables, such as alumina for a solid engine,
- the physical properties of mixture (C_p, γ, Mw, μ, Pr) according to the temperature.

Among those results, only the following are useful for the other modules :

1. mass fraction and physical properties of the condensed phase (TPPLUME) ;
2. table of the physical and thermodynamic properties of the gaseous mixture according to the temperature, under the frozen hypothesis (SESJET, MATFLOW, NAVIER, MATPLIMP) ;

The functions of these gas tables are :

according to :

- the static pressure (during the expansion).

compute :

- the enthalpy,
- the ratio of specific heats : $\gamma=C_p/C_v$,
- the temperature,
- the specific heat C_p of the mixture,
- the dynamic viscosity : μ,

- the Prandtl number : Pr.

Those tables are calculated with the assumption of frozen concentrations.

The freezing point can be defined by the user, by specifying the freezing pressure ratio : $P_{chamber} / P_{freezing}$.

1. averaged value of the specific heat C_p and the ratio of specific heat : $\gamma = C_p/C_v$ corresponding to conditions at infinity expansion.
2. table of thermodynamic characteristics of species or group of species (cross section, number of degrees of freedom) dedicated to the Monte-Carlo software (MCLIP, …).

The other results, such as the theoretical rocket performance, are given just for information. The ratio of expansion in the nozzle is not used in the rest of the software (the exact nozzle shape will required by TPPLUME or SESJET).

The chemical composition of the combustion products is locally used by ODE to compute the physical and thermodynamic mixture properties, and not in the rest of the PLUME software.

3.2 METHOD OF ANALYSIS

The chemical equilibrium composition of the propellant system is usually computed by the method of minimization of the Gibbs free energy, under a given thermodynamic state.

An initial estimate is made for the combustion temperature (3800 K) and the composition (molar fractions) and a descent Newton-Raphson method is used to calculate iteratively equilibrium concentrations.

Afterwards, the code computes the flow parameters (P, ρ, T, V), the engine performance and the chemical composition of the combustion products at each nozzle station, assuming either local chemical equilibrium or frozen composition.

Finally, the viscosity and the thermal conductivity are calculated for each species and then combined to give their value for the mixture.

3.3 SOFTWARE LIMITATIONS

The ODE program has no limitation due to its calculation method. The original assumptions of ODE are rigorous.

The main limitations of ODE are linked to the non-exhaustive contents of the database, but for the standard engines, there is no problem.

An other limitation concerns the field of validity of the tabulations of the thermodynamic properties (JANNAF.THE). Actually, they are only valid for temperatures between 300 and 5000 K, or down to 250 K with an extrapolation.

The species list of the JANNAF.THE file is given on Figure 4.3-8 at the end of this document.

4 ODE INPUT / OUTPUT

4.1 ODE ARCHITECTURE

The ODE input files are :

File	Function
JANNAF.THE	Database of thermodynamic properties.
"thruster name".ODI	User input file.

The ODE output files are :

File	Function
"thruster name".T08	Interface file to TPPLUME
"thruster name".THERMO	Frozen gas tables : H, W_{mol}, γ, T, P, C_p, μ, Pr.
"thruster name".T07	Species characteristics for Monte-Carlo calculation
"thruster name".ODO	Output listing file.

All these files are represented on Figure 4.1-1.

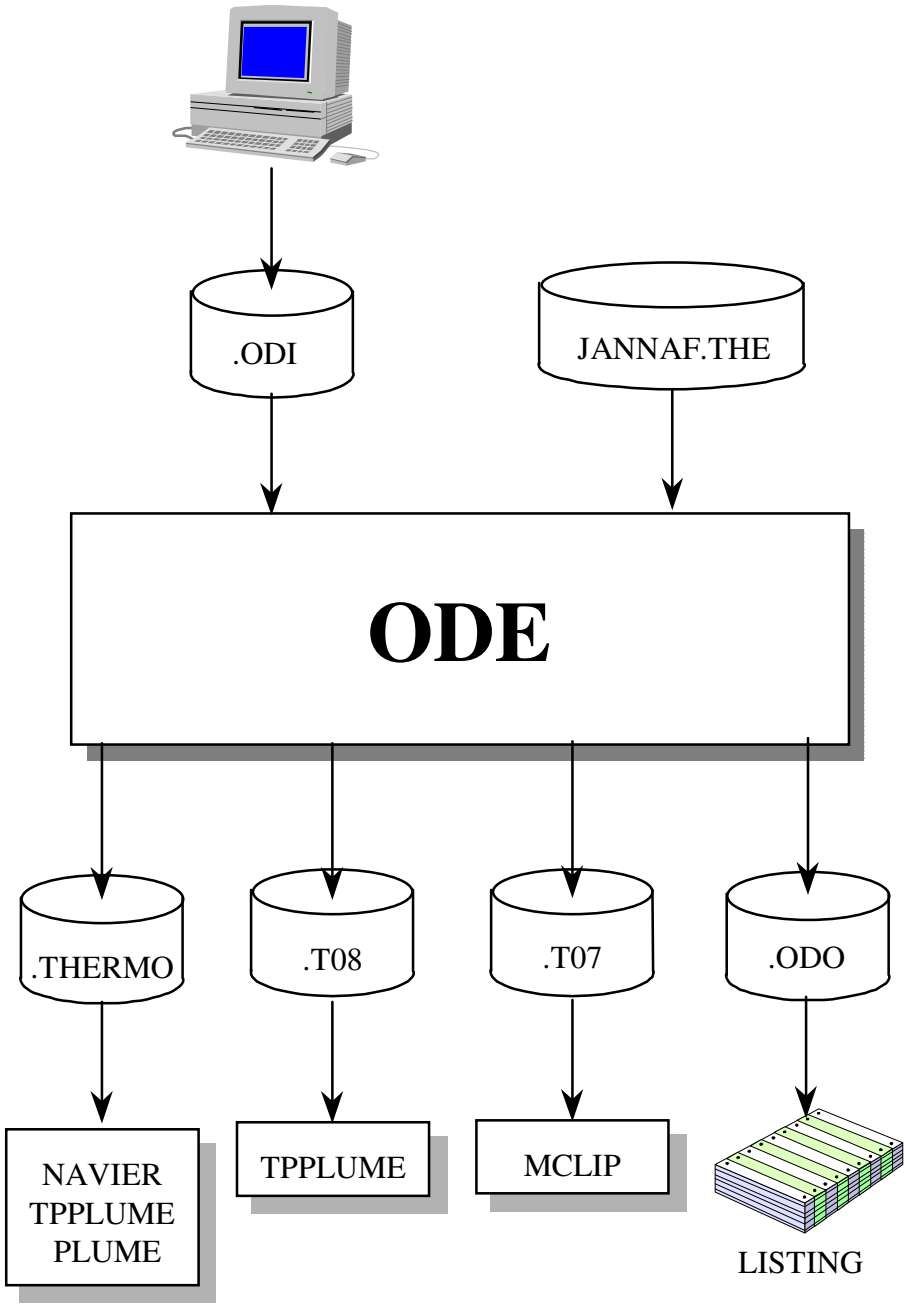

Figure 4.1-1 : architecture of ODE.

4.2 ODE INPUT FILES DESCRIPTION

4.2.1 JANNAF.THE

This is a table including the thermodynamic properties of about 700 chemical species. It is delivered with the software and the user cannot modify it.

The species list is given at the end of the chapter (see Figure 4.3-8).

4.2.2 .ODI file

This is the data file of ODE.

As shown on Figure 4.2-1**,** it is composed of three zones :

zone 1 : Titles,

zone 2 : Reactant definitions,

zone 3 : Namelist ODEM.

zone1 :

The user can define several TITLE cards, which are imperatively at the top of the file.

The syntax of a TITLE card is following :

TITLE text input by the user

The TITLE symbol must be on the left, on the first column. The user has 72 characters to write his text.

The end of the TITLE zone is defined by the card :

XQT

The symbol XQT must be on the left, on the first column.

zone 2 :

The propellants are considered as a mixture of several reactants (up to 15). Each reactant is defined in the input file by one card.

A reactant can be a single species, defined by its chemical formula (ex : N2H4 for hydrazine), or a mixture of several species, defined by its composition in atoms. In both cases, it cannot be composed of more than 5 atoms.

The physico-chemical properties of each reactant are defined as follows.

The reactant specification is introduced by the card :

REACTANTS

This card is just after the card XQT.

On each reactant card there must be first the chemical definition of the species (chemical formula or atom composition) :

CHEMICAL FORMULA ex : N_2O_4, $C_1H_6N_2$, O_2, H_2, AL_1, etc...

ATOM COMPOSITION ex : $N_{0.78}$ $O_{0.22}$ for the air

It can be noticed that the monatomic species must be defined by the atom chemical symbol followed by the number 1 (ex AL_1 for aluminium).

Then the following properties must be defined :

- reactant nature (fuel or oxidant),
- reactant phase (liquid, solid, gas),
- enthalpy of formation of reactant at reference temperature, (in cal/mole),
- reference temperature in Kelvin,
- mass fraction or molar fraction of this reactant with regard to the total value for reactants of the same nature (oxidant or fuel).

These properties are introduced by key-words (see the following array), separated by blanks. All key-words must have at least three characters; their order does not matter.

Definition of the key-words :

Parameter	Key-word	Default value
Nature	OXID/FUEL	FUEL
Phase	GAS, LIQUID, SOLID	GAS
Enthalpy	ENTH=enth	ENTH=0 cal/mole
Temperature	TEMP=temp	TEMP=298.15 K
Mass fraction	FMA=fma	FMA=1
Mole fraction	FMO=fmo	FMO=1

remarks :

- on the same card, FMO and FMA must not appear together.
- if the fuel (or the oxidant) is composed of one of the reactant, it is not necessary to define FMO or FMA. The default value is 1.
- the enthalpy of formation of an element is zero at 298.15 K.
- if the user does not know the enthalpy, he can ask the program to look at the thermodynamic file JANNAF.THE. In that case, the key-word LOOK will replace ENTH=enth. He must also check that the reactant is in JANNAF.THE, under the same phase.

example :

N_2O_4 OXID GAS LOOK

The end of the reactant data is noticed by the card :

END

remark :

In the case of monopropellant motors, (hydrazine N_2H_4 for example), ODE considers the propellant as a fuel, whatever the user has specified for the propellant in ODE input (OXID or FUEL).

In the case of solid motors, the reactants are sometimes difficult to characterize in a detailed manner. But, if the propellant elemental composition and enthalpy of formation are known, the user can proceed as follows :

- each reactant is considered as an element (AL_1, C_1...) of fuel nature,
- the whole propellant enthalpy is assigned to the first reactant with a proportional correction :

$$ENTH = \frac{\Delta H.W_m}{Fmol(1)}$$

where : ENTH : enthalpy to be assigned to the first reactant, (in cal/mole),

ΔH : enthalpy produced by the burning propellant, (in cal/g),

W_m : molecular weight of the propellant, (in g/mole),

F_{mol} (1) : molar fraction of the first reactant.

Note that :

$$W_m = \sum_i Fmol(1).W_m(1)$$

where : $F_{mol}(i)$: molar fraction of the component *i*

$W_m(i)$: molecular weight of the component *i*

Example of input file on Figure 4.2-1for the solid motor MAGE II AKM.

zone 3 :

Namelist ODEM, introduced by the card NAMELISTS and described on the following pages.

4.2.2.1 Namelist $ODEM

Purpose

To specify the control parameters for ODE.

Format of the file

```
$ODEM

PC = pc        [TC=tc]          OFC = ofc
[OF=of]        [ERATIO=eratio]  [FPCT=fpct]
[FA=fa]        [SOLPT=solpt]    [LISTSP=listsp]
SUBAR=subar    SUPAR =supar     [IVA=iva]
[QPR=qpr]
$END
```

Description

PC — specifies the chamber pressure in bar.

Type : real

Range : >0

TC — specifies the combustion temperature in Kelvin

Type : real

Range : >0

Default : computed by the software as the adiabatic combustion temperature

OFC — specifies the value of the oxidant/fuel ratio.

Type : real

Range : >0

OF — specifies whether OFC is the oxidant/fuel weight ratio.

Range : T, F

Default : F

ERATIO — specifies whether OFC is the equivalent ratio (ratio between mixing ratio and stoichiometric mixing ratio)

Range : T, F

Default : F

FCPT — specifies whether OFC is the percentage of fuel by weight.

Range : T, F

Default : F

FA — specifies whether OFC is the fuel/oxidant weight ratio.

Range : T, F

Default : F

SOLPT — specifies, for solid thruster, whether the solidification point of the condensed species will be computed.

Range : T, F

Default : F

LISTP — specifies whether the list of the species available in the JANNAF.THE will be printed.

Range : T, F

Default : F

SUBAR — specifies the subsonic area ratios for rocket performance computation, normalized by the throat section.

Type : real

Range : >1

Note : up to 13 values can be specified, separated by commas

SUPAR specifies the supersonic area for rocket performance computation, normalized by the throat section.

Type : real

Range : >1

Note : up to 50 values can be specified, separated by commas

IVA specifies the number of lines of the gas table.

Type : integer

Range : >2

Default : 12

QPR specifies the pressure ratio between two table lines.

Type : real

Range : >1

Default : 2

```
TITLE   TELECOM-1  A.K.M.  (MAGE II)
XQT
REACTANTS
AL1    FUEL   SOL     FMOL =  5.9323     ENTH =-56200
H1     FUEL   SOL     FMOL = 38.3847
C1     FUEL   SOL     FMOL =  8.6494
N1     FUEL   SOL     FMOL =  6.1276
O1     FUEL   SOL     FMOL = 24.610
CL1    FUEL   SOL     FMOL =  6.1276
END
NAMELISTS
 $ODEM
   PC    = 35.7 ,
   FPCT  = T ,
   OFC   = 100. ,
   SUBAR = 3.46 ,
   SUPAR = 2 , 50 , 65 ,
   IVA   = 10 , QPR = 4
   LISTSP = F
   SOLPT = T ,
 $END
```

Figure 4.2-1 : AKM.ODI : example of input file for ODE.

4.3 ODE INPUT FILES DESCRIPTION

All the output files can be edited. They are described below :

4.3.1 .T08 file

This file transfers ODE results to TPPLUME.

4.3.2 .THERMO file

This is an interface file to SESJET, NAVIER MATFLOW and PLUME.

It contains a table giving, versus the temperature : H, W_{mol}, γ, T, P, C_p, μ, Pr.

4.3.3 .T07 file

This is an interface file to MCLIP and CONTAMINE.

It contains the species characteristics : collisional cross sections, number of degrees of freedom.

4.3.4 .ODO file

This is the output listing file of ODE. Its contents is now presented :

1. review of the parameters (see Figure 4.3-1) :
   - list of reactants : with :

     FRAC : molar fraction, if MOL=T.

     mass fraction, if MOL=F.

     STATE : the state of the reactant.

     FOX : the reactant nature : O for oxidant,

     F for fuel.

     TEMP : the temperature for which ENTH is computed.

     The other parameters are described in the Input data section.
   - namelist ODEM :

     All these variables are described in the Input data section.
2. list of chemical species considered in this system (see Figure 4.3-2) :

   They come from the file JANNAF.THE.

3. contents of the file "thruster name".THERMO :

   It is a gas properties tabulation versus temperature assuming a frozen expansion (see Figure 4.3-3).

4. theoretical rocket performance assuming equilibrium composition (see Figure 4.3-4) :

   - Thermo-physical properties of the mixture at different locations in the nozzle :

     list of parameters :

     PC/P : ratio of chamber pressure to static pressure

     P : static pressure

     T : static temperature

     H : enthalpy

     S : entropy

     DEN : density

     M : molar weight

     $(DLV/DLP)_T$:partial derivative $(\partial \log V / \partial \log P)_T$

     $(DLV/DLT)_P$:partial derivative $(\partial \log V / \partial \log P)_P$

     C_p : specific heat at constant pressure

     γ (S) : isentropic exponent : $(\partial \log P / \partial \log r)_S$

     SON VEL : sound velocity : $a = (\partial P / \partial lr)_S$

     MACH NUMBER : Mach number : M = V/a

     VEL : gas velocity : $V = \sqrt{2(H - H_0)}$

     AE/AT : expansion ratio : (A_{exit}/A_{throat})

     CSTAR : characteristic velocity : $C^*=P_c/(\rho V)_{throat}$

     CF : thrust coefficient : V/C*

     IVAC : specific impulse in the vacuum : IVAC=(V+pA/m)/g with $g=9.81 m/s^2$

     I : specific impulse when $P_{exit}=P_{amb}$: I=V/g

     note : an additional column (PC/P=0) corresponds to the solidification point of alumina (computed if SOLPT=T).

   - Molar fractions of all the species at the same locations (**see Figure 4.3-5**)
   - Mass fractions of total condensables (**see Figure 4.3-5**)

   The variation of condensed mass fraction is transmitted to TPPLUME (with thermo-physical properties of the condensed phase) for a two phase computation.

5. Frozen transport properties calculated from equilibrium concentrations :

   values of : μ (viscosity),

   k (thermal conductivity),

   Pr (Prandtl number),

   at several locations : chamber, throat, exit (see Figure 4.3-6).

6. theoretical rocket performance assuming frozen composition (see Figure 4.3-7)

   Mixture thermo-physical properties at different locations in the nozzle : These parameters have been described for the equilibrium composition.

   comments : in the case of a frozen chemistry, the molecular weight M is constant and γ is computed by the relation :

$$\gamma = \frac{Cp}{Cv} = \frac{Cp}{Cp - R} \quad \text{and} \quad R = \frac{8314}{M} \quad \text{in J/Kg/K}$$

   remark : for a solid motor, there would be computations for another location corresponding to the particle solidification point.

Hereafter, is the listing in the case of the motor MAGE II : AKM.

```
------------------------------------------------------------------------------------------------------------------------------------------
------
         TITLE OF ODE INPUT FILE :      TELECOM-1  A.K.M.  (MAGE II)                                                    DATE : 12-DEC-
90
------------------------------------------------------------------------------------------------------------------------------------------
------


REACTANTS
---------

CHEMICAL : AL  1.0000
FRAC= 5.93230  MOL=T  ENTH=-0.5620E+05  STATE=S  FOX=F  LOOK=F  TEMP=  298.1

CHEMICAL : H   1.0000
FRAC=38.38470  MOL=T  ENTH= 0.0000E+00  STATE=S  FOX=F  LOOK=F  TEMP=  298.1

CHEMICAL : C   1.0000
FRAC= 8.64940  MOL=T  ENTH= 0.0000E+00  STATE=S  FOX=F  LOOK=F  TEMP=  298.1

CHEMICAL : N   1.0000
FRAC= 6.12760  MOL=T  ENTH= 0.0000E+00  STATE=S  FOX=F  LOOK=F  TEMP=  298.1

CHEMICAL : O   1.0000
FRAC=24.61000  MOL=T  ENTH= 0.0000E+00  STATE=S  FOX=F  LOOK=F  TEMP=  298.1

CHEMICAL : CL  1.0000
FRAC= 6.12760  MOL=T  ENTH= 0.0000E+00  STATE=S  FOX=F  LOOK=F  TEMP=  298.1




NAMELISTS
---------


chamber temperature determined by the adiabatic combustion

chamber pressure (BARS)              PC =   35.7000

percent fuel by weight              OFC =    100.00


subsonic area ratios              SUBAR =     3.460

supersonic area ratios            SUPAR =     2.000      50.000      65.000

ratio of pressure between           QPR =      4.00
2 lines of the gas table

number of lines of the gas table    IVA =        10

ratio of pressure PC/P             QFRZ =      1.00
of freezing point

calculate the solidification      SOLPT =      TRUE
point of particles

     NO $ODE VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT
```

Figure 4.3-1 : AKM.ODO : review of the input data

```
------------------------------------------------------------------------------------------------------------------------
------
        TITLE OF ODE INPUT FILE :      TELECOM-1  A.K.M.  (MAGE II)                                        DATE : 12-DEC-
90
------------------------------------------------------------------------------------------------------------------------
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SPECIES BEING CONSIDERED IN THIS SYSTEM
---------------------------------------

    J12/65  AL(S)            J12/65  AL(L)            J12/65  AL               J 6/70  ALCL             J 6/72  ALCL2
    J 6/70  ALCL3(S)         J 6/70  ALCL3(L)         J 6/70  ALCL3            J 6/63  ALH              J12/62  ALN(S)
    J 3/67  ALN              J 6/75  ALO              J 9/64  ALOCL            J12/67  ALOH             J12/75  ALO2
    J12/68  ALO2H            J 6/70  AL2CL6           J 6/75  AL2O             J12/75  AL2O2            J 6/75  AL2O3(S)
    J 6/75  AL2O3(L)         J 3/61  C(S)             J 3/61  C                J12/69  CCL              J12/68  CCL2
    J 6/70  CCL3             J12/68  CCL4            J12/67  CH               J12/72  CH2              J 3/61  CH2O
    J 6/69  CH3              J 3/61  CH4             J 6/69  CN               J 6/66  CNN              J12/70  CN2
    J 9/65  CO               J12/65  COCL            J 6/61  COCL2            J 9/65  CO2              J12/69  C2
    J12/68  C2CL2            J 3/67  C2H             J 3/61  C2H2             J 9/65  C2H4             L 5/72  C2H6
    J 3/67  C2N              J 3/61  C2N2            J 9/66  C2O              J12/69  C3               J 6/68  C3O2
    J12/69  C4               J12/69  C5              J 6/72  CL               J 6/66  CLCN             J 6/61  CLO
    J 3/61  CLO2             J 9/65  CL2             J12/65  CL2O             J 6/74  H                J 3/64  HALO
    J 9/64  HCL              L12/69  HCN             J12/70  HCO              J12/70  HNCO             J 3/63  HNO
    J 6/63  HNO2             J 6/63  HNO3            J 3/64  HO2              J 3/61  H2               L11/65  H2O(S)
    L11/65  H2O(L)           J 3/61  H2O             L 2/69  H2O2             J 3/61  N                J12/70  NCO
    J12/71  NH               J12/65  NH2             J 9/65  NH3              J 6/63  NO               J12/72  NOCL
    J 9/64  NO2              J12/65  NO2CL           J12/64  NO3              J 9/65  N2               J12/65  N2H4
    J12/64  N2O              J 9/64  N2O4            J12/64  N2O5             J12/70  N3               J 6/74  O
    J12/70  OH               J 9/65  O2              J 6/61  O3
```

Figure 4.3-2 : AKM.ODO : list of the species

```
------------------------------------------------------------------------------------------------------------------------
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        TITLE OF ODE INPUT FILE :      TELECOM-1  A.K.M.  (MAGE II)                                        DATE : 12-DEC-
90
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   FROZEN TABLES


         NUMBER OF EXPANSION STEPS : IVA  = 10

         PRESSURE DIMINUTION RATIO : QPR  =  4.00

         PC/P OF FREEZING POINT    : QFRZ =  1.00



  H (J/KG)       WMOL      GAMMA    T (DEG K)   P (PA)       CP(SI)     MU (SI)       PR

0.23373E+07     20.050    1.24986    4661.04  0.14280E+08   2074.296  0.11368E-03   0.470251
0.00000E+00     20.050    1.25883    3518.90  0.35700E+07   2016.748  0.94768E-04   0.471652
-.17577E+07     20.050    1.26977    2634.31  0.89250E+06   1951.822  0.78181E-04   0.472881
-.30670E+07     20.050    1.28544    1949.95  0.22313E+06   1867.410  0.63765E-04   0.472549
-.40294E+07     20.050    1.30677    1421.20  0.55781E+05   1766.417  0.51066E-04   0.469351
-.47246E+07     20.050    1.33323    1015.89  0.13945E+05   1659.064  0.40075E-04   0.463416
-.52165E+07     20.050    1.35962     710.97  0.34863E+04   1567.741  0.30687E-04   0.452981
-.55579E+07     20.050    1.37859     488.99  0.87158E+03   1509.968  0.22840E-04   0.441296
-.57913E+07     20.050    1.38969     332.70  0.21790E+03   1478.786  0.16667E-04   0.432445
-.62833E+07     20.050    1.38969       0.00  0.00000E+00   1478.786  0.00000E+00   0.432445



         EXPANSION-AVERAGED CP AND GAMMA
         -------------------------------

         CP =   1785.589     GAMMA =    1.30248
```

Figure 4.3-3 : AKM.ODO : gas table (contents of .THERMO)

```
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         TITLE OF ODE INPUT FILE :      TELECOM-1  A.K.M.  (MAGE II)                                                    DATE : 12-DEC-
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                    THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC =  35.700 BAR
                CHAMBER    THROAT      EXIT      EXIT      EXIT      EXIT      EXIT
PC/P             1.0000    1.7296    0.0000    1.0174    7.5884    497.10    694.04
P, BAR            35.70     20.64    0.7802     35.09     4.705    0.0718    0.0514
T, DEG K           3519      3336      2327      3513      2868      1751      1658
H, CAL/G         -333.6    -466.7   -1105.6    -337.9    -786.5   -1443.7   -1482.2
S, CAL/(G)(K)    2.3561    2.3561    2.3561    2.3561    2.3561    2.3561    2.3561
DEN (KG/M**3)   3.40210   2.09570   0.11803   3.35071   0.56803   0.01451   0.01098

M, MOL WT        27.879    28.155    29.267    27.888    28.792    29.412    29.417
(DLV/DLP)T     -1.02730  -1.02215  -1.00265  -1.02712  -1.01081  -1.00018  -1.00009
(DLV/DLT)P       1.4737    1.4007    1.0636    1.4714    1.2196    1.0056    1.0029
CP, CAL/(G)(K)   1.0821    1.0042    0.5675    1.0796    0.7871    0.4219    0.4146
GAMMA (S)        1.1309    1.1309    1.1530    1.1309    1.1358    1.1929    1.1959
SON VEL,M/SEC    1089.4    1055.4     873.1    1088.3     969.9     768.3     748.7
MACH NUMBER      0.0000    1.0000    2.9112    0.1751    2.0072    3.9669    4.1411
VEL,M/S              0.     1055.     2542.      191.     1947.     3048.     3100.

AE/AT                       1.0000    7.3732    3.4637    2.0000    50.001    65.001
CSTAR, M/SEC                 1614.     1614.     1614.     1614.     1614.     1614.
CF                           0.654     1.575     0.118     1.206     1.888     1.921
IVAC, (SEC)                  202.8     285.7     579.8     241.9     327.4     331.6
I, (SEC)                     107.6     259.2      19.4     198.5     310.8     316.1


MOL WT(MIX)      25.891    26.083    26.930    25.897    26.551    27.051    27.055
```

Figure 4.3-4 : AKM.ODO : theoretical rocket performance assuming equilibrium composition

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MOLE FRACTIONS


AL              0.000189 0.000097 0.000000 0.000185 0.000009 0.000000 0.000000
ALCL            0.004967 0.003459 0.000048 0.004915 0.000877 0.000000 0.000000
ALCL2           0.001406 0.001003 0.000027 0.001392 0.000297 0.000000 0.000000
ALCL3           0.000097 0.000077 0.000008 0.000096 0.000035 0.000000 0.000000
ALH             0.000022 0.000010 0.000000 0.000021 0.000001 0.000000 0.000000
ALO             0.000409 0.000208 0.000000 0.000401 0.000018 0.000000 0.000000
ALOCL           0.002150 0.001576 0.000034 0.002131 0.000472 0.000000 0.000000
ALOH            0.000541 0.000346 0.000003 0.000534 0.000070 0.000000 0.000000
ALO2            0.000087 0.000044 0.000000 0.000085 0.000004 0.000000 0.000000
ALO2H           0.001044 0.000689 0.000007 0.001031 0.000152 0.000000 0.000000
NO              0.001260 0.000871 0.000020 0.001247 0.000242 0.000000 0.000000
N2              0.078720 0.079509 0.082541 0.078746 0.081268 0.082923 0.082936
O               0.001809 0.001192 0.000010 0.001787 0.000257 0.000000 0.000000
OH              0.015102 0.011592 0.000645 0.014985 0.004472 0.000015 0.000006
O2              0.000471 0.000311 0.000003 0.000465 0.000068 0.000000 0.000000

AL(S)           0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
AL(L)           0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
ALCL3(S)        0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
ALCL3(L)        0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
ALN(S)          0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
ALN             1.73E-08 0.00E+00 0.00E+00 1.67E-08 0.00E+00 0.00E+00 0.00E+00
N2H4            0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
N2O             1.28E-07 6.71E-08 0.00E+00 1.26E-07 0.00E+00 0.00E+00 0.00E+00
N2O4            0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
N2O5            0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
N3              0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
O3              0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
MASS FRACTION OF TOTAL CONDENSIBLES
------------------------------------
CONDENSIBLES    0.280816 0.287797 0.302355 0.281064 0.298875 0.302596 0.302596
MOLECULAR WEIGHT OF TOTAL CONDENSIBLES IN THE CHAMBER=    101.9612
GAS MOLECULAR WT IN THE CHAMBER=     20.0503
EROSION PARAMETER BETA=      0.34060
```

Figure 4.3-5 : AKM.ODO : molar fractions

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        TITLE OF ODE INPUT FILE :      TELECOM-1  A.K.M.  (MAGE II)                                                                    DATE : 12-
DEC-90
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                        FROZEN TRANSPORT PROPERTIES CALCULATED FROM EQUILIBRIUM CONCENTRATIONS

     STATION                   MU                  K                   PR
                            (N-SEC/M**2)       (N/SEC-DEG K)
     CHAMBER              0.94767849E-04      0.41040704E+00      0.47165114E+00
     THROAT               0.91475595E-04      0.39472419E+00      0.47377506E+00
     EXIT                 0.57003632E-04      0.24413325E+00      0.47816068E+00
    VISCOSITY EXPONENT (OMEGA) FOR THE FORM MU=MUREF*(T/TREF)**OMEGA IS     0.67664
    MUREF FOR INPUT TO TPPLUME=   0.94848328E-04 N-SEC/M**2
          SPECIES CONSIDERED IN TRANSPORT PROPERTIES CALCULATIONS
          AL                  ALCL                ALCL3               ALN
          ALO                 C                   CCL                 CCL2
          CCL3                CCL4                CH                  CH4
          CN                  CO                  CO2                 C2
          C2H2                C2H4                C2H6                C2N2
          CL                  CLCN                CLO                 CL2
          H                   HCL                 HCN                 H2
          H2O                 H2O2                N                   NH
          NH3                 NO                  NOCL                N2
          N2O                 O                   OH                  O2
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Figure 4.3-6 : AKM.ODO : frozen transport properties

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        TITLE OF ODE INPUT FILE :      TELECOM-1  A.K.M.  (MAGE II)                                                    DATE : 12-DEC-
90
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                        THEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN COMPOSITION DURING EXPANSION

PC =  35.700 BAR
                CHAMBER   THROAT     EXIT     EXIT     EXIT     EXIT
PC/P             1.0000   1.7586   1.0181   8.0788   610.18   851.02
P, BAR            35.70    20.30    35.07    4.419   0.0585   0.0419
T, DEG K           3519     3231     3509     2559     1277     1207
H, CAL/G         -333.6   -469.3   -338.1   -782.6  -1353.7  -1383.2
S, CAL/(G)(K)    2.3561   2.3561   2.3561   2.3561   2.3561   2.3561
DEN (KG/M**3)    3.40210  2.10676  3.35079  0.57912  0.01537  0.01166

M, MOL WT         27.879   27.879   27.879   27.879   27.879   27.879
CP, CAL/(G)(K)    0.4733   0.4703   0.4733   0.4609   0.4243   0.4212
GAMMA (S)         1.1773   1.1786   1.1773   1.1829   1.2019   1.2037
SON VEL,M/SEC     1111.5   1065.7   1110.0    950.1    676.4    658.2
MACH NUMBER       0.0000   1.0000   0.1745   2.0403   4.3193   4.5025
VEL,M/S               0.     1066.     194.    1938.    2922.    2964.

AE/AT                    1.0000   3.4597   2.0000   50.000   65.000
CSTAR, M/SEC              1590.    1590.    1590.    1590.    1590.
CF                        0.670    0.122    1.219    1.837    1.864
IVAC, (SEC)               200.9    570.8    237.8    311.2    314.6
I, (SEC)                  108.7     19.7    197.7    297.9    302.2


MOLE FRACTIONS

AL          0.000189      ALCL        0.004967      ALCL2       0.001406      ALCL3       0.000097
ALH         0.000022      ALO         0.000409      ALOCL       0.002150      ALOH        0.000541
ALO2        0.000087      ALO2H       0.001044      AL2O        0.000060      AL2O2       0.000015
AL2O3(L)    0.071308      CH2O        0.000001      CO          0.207077      COCL        0.000009
CO2         0.016955      CL          0.017565      CLO         0.000018      CL2         0.000028
H           0.048809      HALO        0.000001      HCL         0.130871      HCN         0.000003
HCO         0.000019      HNO         0.000002      HO2         0.000002      H2          0.240956
H2O         0.157996      H2O2        0.000001      N           0.000011      NH          0.000004
NH2         0.000010      NH3         0.000006      NO          0.001260      N2          0.078720
O           0.001809      OH          0.015102      O2          0.000471
ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .0000005 FOR ALL ASSIGNED CONDITIONS


AL(S)       AL(L)       ALCL3(S)    ALCL3(L)    ALN(S)      ALN         AL2CL6      C(S)        C           CCL
CCL2        CCL3        CCL4        CH          CH2         CH3         CH4         CN          CNN         CN2
COCL2       C2          C2CL2       C2H         C2H2        C2H4        C2H6        C2N         C2N2        C2O
C3          C3O2        C4          C5          CLCN        CLO2        CL2O        HNCO        HNO2        HNO3
H2O(S)      H2O(L)      NCO         NOCL        NO2         NO2CL       NO3         N2H4        N2O         N2O4
N2O5        N3          O3
```

Figure 4.3-7 : AKM.ODO : theoretical rocket performance assuming frozen composition

1	J12/65	AL(S)	62	J12/64	B(L)
2	J12/65	AL(L)	63	J12/64	B
3	J12/65	AZ(S)	64	J12/70	B+
4	J12/65	AZ(L)	65	J12/64	BCL
5	J12/65	AL	66	J 6/68	BCL+
6	J 6/65	AL+	67	J12/64	BCLF
7	J 6/66	ALBO2	68	J 6/72	BCL2
8	J 6/72	ALBR	69	J12/70	BCL2+
9	J 6/72	ALBR3(S)	70	J 6/72	BCL2-
10	J 6/72	ALBR3(L)	71	J12/64	BCL3
11	J 6/72	ALBR3	72	J12/64	BF
12	J 6/70	ALCL	73	J 6/72	BF2
13	J 6/70	ALCL+	74	J12/70	BF2+
14	J 9/64	ALCLF	75	J 6/72	BF2-
15	J 9/64	ALCLF2	76	J 6/69	BF3
16	J 6/72	ALCL2	77	J12/64	BH
17	J 6/72	ALCL2+	78	J12/65	BHF2
18	J 6/72	ALCL2-	79	J12/64	BH2
19	J 9/64	ALCL2F	80	J12/64	BH3
20	J 6/70	ALCL3(S)	81	J 6/66	BN(S)
21	J 6/70	ALCL3(L)	82	J 6/66	BN
22	J 6/70	ALCL3	83	J 6/68	BO
23	J12/75	ALF	84	J 3/65	BOCL
24	J12/75	ALF+	85	J 3/65	BOF
25	J 6/72	ALF2	86	J12/66	BOF2
26	J 6/72	ALF2+	87	J 6/68	BO2
27	J 6/72	ALF2-	88	J12/68	BO2-
28	J 6/70	ALF3(S)	89	J 6/72	BS
29	J 6/70	ALF3(S)	90	J12/64	B2
30	J 6/70	ALF3	91	J 6/66	B2O
31	J 6/63	ALH	92	J12/64	B2O2
32	J 9/64	ALI	93	J 6/71	B2O3(L)
33	J 6/64	ALI3(S)	94	J 6/71	B2O3
34	J 6/64	ALI3(L)	95	J 3/65	B3O3CL3
35	J 6/64	ALI3	96	J 3/65	B3O3F3
36	J12/62	ALN(S)	97	J12/70	BA(S)
37	J 3/67	ALN	98	J12/70	BA(S)
38	J 6/75	ALO	99	J12/70	BA(S)
39	J 6/75	ALO+	100	J12/70	BA(L)
40	J 12/7	ALO-	101	J12/70	BA
41	J 9/64	ALOCL	102	J12/74	BABR
42	J12/75	ALOF	103	J12/74	BABR2(S)
43	J12/67	ALOH	104	J12/74	BABR2(L)
44	J12/67	ALOH+	105	J12/74	BABR2
45	J12/67	ALOH-	106	J12/72	BACL
46	J12/75	ALO2	107	J12/72	BACL2(S)
47	J12/75	ALO2-	108	J12/72	BACL2(S)
48	J12/68	ALO2H	109	J12/72	BACL2(L)
49	J 6/72	AL2BR6	110	J12/72	BACL2
50	J 6/70	AL2CL6	111	J12/72	BAF
51	J 6/70	AL2F6	112	J12/72	BAF+
52	J 3/63	AL2MGO4(S)	113	J12/72	BAF2(S)
53	J 6/75	AL2O	114	J12/72	BAF2(S)
54	J 6/75	AL2O+	115	J12/72	BAF2(L)
55	J12/75	AL2O2	116	J12/72	BAF2
56	J12/75	AL2O2+	117	J 6/74	BAO(S)
57	J 6/75	AL2O3(S)	118	J 6/74	BAO(L)
58	J 6/75	AL2O3(L)	119	J12/75	BAOH
59	L 5/66	AR	120	J12/75	BAO2H2(S)
60	L12/66	AR+	121	J12/75	BAO2H2(L)
61	J12/64	B(S)	122	J12/75	BAO2H2

Figure 4.3-8 : list of the JANNAF.THE species.

123	J 9/61	BE(S)	184	J12/67	CH
124	J 9/61	BE(L)	185	J12/71	CH+
125	J 9/61	BE	186	J12/72	CH2
126	J 6/65	BE+	187	J 3/61	CH2O
127	J 6/66	BEBO2	188	J 6/69	CH3
128	J 6/75	BEBR	189	J 3/61	CH4
129	J 6/75	BEBR2(S)	190	J 6/69	CN
130	J 6/75	BEBR2	191	J12/70	CN+
131	J 9/66	BECL	192	J12/70	CN-
132	J 6/68	BECL+	193	J 6/66	CNN
133	J 6/65	BECLF	194	J12/70	CN2
134	J 6/65	BECL2(S)	195	J 9/65	CO
135	J 6/65	BECL2(L)	196	J12/65	COCL
136	J 6/65	BECL2	197	J 6/61	COCL2
137	J12/71	BEF	198	J12/65	COF
138	J 6/70	BEF2(S)	199	J12/69	COF2
139	J 6/70	BEF2(S)	200	J 3/61	COS
140	J 6/70	BEF2(L)	201	J 9/65	CO2
141	J 6/70	BEF2	202	J12/66	CO2-
142	J 3/63	BEH	203	J 6/62	CP
143	J 9/66	BEH+	204	J12/62	CS
144	J12/75	BEI	205	J 6/61	CS2
145	J12/75	BEI2(S)	206	J12/64	CZR(S)
146	J12/75	BEI2(L)	207	J12/64	CZR(L)
147	J12/75	BEI2	208	J12/69	C2
148	J 6/63	BEN	209	J12/69	C2-
149	J 6/75	BEO(S)	210	J12/68	C2CL2
150	J 6/75	BEO(L)	211	J12/67	C2F2
151	J12/74	BEO	212	J 6/69	C2F4
152	J12/75	BEOH	213	J 3/67	C2H
153	J12/75	BEOH+	214	J12/67	C2HF
154	J12/75	BEO2H2(S)	215	J 3/61	C2H2
155	J 12/7	BEO2H2	216	J 9/65	C2H4
156	J 9/63	BE2O	217	L 5/72	C2H6
157	J 6/66	BE2OF2	218	J 3/67	C2N
158	J 9/63	BE2O2	219	J 3/61	C2N2
159	J 9/63	BE3O3	220	J 9/66	C2O
160	J 9/63	BE4O4	221	J12/69	C3
161	BAR 73	BI(S)	222	J 6/68	C3O2
162	BAR 73	BI(L)	223	J12/69	C4
163	L 7/75	BI	224	J12/69	C5
164	L 7/75	BIS	225	J12/68	CA(S)
165	L 8/76	BI2S3(S)	226	J12/68	CA(S)
166	J 6/74	BR	227	J12/68	CA(L)
167	J 9/61	BR2(L)	228	J12/68	CA
168	J12/61	BR2	229	J12/70	CA+
169	J 3/61	C(S)	230	J12/74	CABR
170	J 3/61	C	231	J 6/74	CABR2(S)
171	L12/66	C+	232	J 6/74	CABR2(L)
172	J 9/65	C-	233	J 6/74	CABR2
173	J12/69	CCL	234	BAR 73	CACO3(S)
174	J12/68	CCL2	235	BAR 73	CACO3(S)
175	J 6/70	CCL3	236	J 6/70	CACL
176	J12/68	CCL4	237	J 6/70	CACL2(S)
177	J 6/70	CF	238	J 6/70	CACL2(L)
178	J12/70	CF+	239	J 6/70	CACL2
179	J 6/70	CF2	240	J12/68	CAF
180	J12/70	CF2+	241	J12/68	CAF2(S)
181	J 6/69	CF3	242	J12/68	CAF2(S)
182	J12/71	CF3+	243	J12/68	CAF2(L)
183	J 6/69	CF4	244	J12/68	CAF2

Figure 4.3-9 (continued): list of the JANNAF.THE species.

245	J 6/74	CAI	306	J12/69	F2O
246	J 6/74	CAI2	307	J 3/65	FE(S)
247	J 6/73	CAO(S)	308	J 3/65	FE(S)
248	J 6/73	CAO(L)	309	J 3/65	FE(S)
249	J12/74	CAO	310	J 3/65	FE(L)
250	J12/75	CAOH	311	J 3/65	FE
251	J12/75	CAOH+	312	J 6/65	FECL
252	J12/75	CAO2H2(S)	313	J12/70	FECL2(S)
253	J 12/7	CAO2H2	314	J12/70	FECL2(L)
254	J12/71	CAS(S)	315	J12/70	FECL2
255	BAR 73	CASO4(S)	316	J 6/65	FECL3(S)
256	J 6/72	CL	317	J 6/65	FECL3(L)
257	J 6/65	CL+	318	J 6/65	FECL3
258	J 6/65	CL-	319	J 6/65	FEO(S)
259	J 6/66	CLCN	320	J 6/65	FEO(L)
260	J 9/65	CLF	321	J 9/66	FEO
261	J 9/65	CLF3	322	J 6/66	FEO2H2(S)
262	J 6/61	CLO	323	J12/66	FEO2H2
263	J 3/61	CLO2	324	J 6/66	FEO3H3(S)
264	J 9/65	CL2	325	BAR 73	FES(S)
265	J12/65	CL2O	326	BAR 73	FES(S)
266	J 6/73	CR(S)	327	BAR 73	FES(S)
267	J 6/73	CR(L)	328	BAR 73	FES(L)
268	J 6/73	CR	329	J 6/66	FESO4(S)
269	J12/73	CRN(S)	330	BAR 73	FES2(S)
270	J12/73	CRN	331	J12/70	FE2CL4
271	J12/73	CRO	332	J 6/65	FE2O3(S)
272	J12/73	CRO2	333	J 6/66	FE2S3O12(S)
273	J12/73	CRO3	334	J 6/65	FE3O4(S)
274	J12/73	CR2N(S)	335	J 6/74	H
275	J12/73	CR2O3(S)	336	J 6/66	H+
276	J12/73	CR2O3(L)	337	J 9/65	H-
277	J 6/68	CS(S)	338	J 3/64	HALO
278	J 6/68	CS(L)	339	J12/75	HBO
279	J 6/68	CS	340	J12/75	HBO+
280	J12/70	CS+	341	J12/75	HBO-
281	J 6/68	CSCL(S)	342	J12/64	HBO2
282	J 6/68	CSCL(S)	343	J12/75	HBS
283	J 6/68	CSCL(L)	344	J12/75	HBS+
284	J 6/68	CSCL	345	J 9/65	HBR
285	J 6/68	CSF(S)	346	J 9/64	HCL
286	J 6/68	CSF(L)	347	L12/69	HCN
287	J 6/68	CSF	348	J12/70	HCO
288	J12/68	CSO	349	J12/70	HCO+
289	J 6/71	CSOH(S)	350	J12/69	HCP
290	J 6/71	CSOH(S)	351	J12/68	HF
291	J 6/71	CSOH(L)	352	J 9/61	HI
292	J 6/71	CSOH	353	J12/70	HNCO
293	J12/71	CSOH+	354	J 3/63	HNO
294	J 6/68	CS2	355	J 6/63	HNO2
295	J 6/68	CS2CL2	356	J 6/63	HNO3
296	J 6/68	CS2F2	357	J12/72	HOF
297	J12/68	CS2O	358	J 3/64	HO2
298	J 6/71	CS2O2H2	359	J 6/72	HSO3F
299	L02/67	E	360	J 3/61	H2
300	J 9/65	F	361	L11/65	H2O(S)
301	J12/71	F-	362	L11/65	H2O(L)
302	J 6/69	FCN	363	J 3/61	H2O
303	J12/66	FO	364	L 2/69	H2O2
304	J 9/66	FO2	365	J12/65	H2S
305	J12/60	F2	366	J12/66	H2SO4(L)

Figure 4.3-10 (continued): list of the JANNAF.THE species.

367	J12/66	H2SO4	428	J12/66	LIN
368	J12/64	H3B3O6	429	J 3/64	LIO
369	L 5/66	HE	430	J12/67	LIO-
370	L12/66	HE+	431	J 6/71	LIOH(S)
371	J12/61	HG(L)	432	J 6/71	LIOH(L)
372	J12/61	HG	433	J 6/71	LIOH
373	J 3/62	HGBR2(S)	434	J12/71	LIOH+
374	J 3/62	HGBR2(L)	435	J 9/66	LION
375	J 3/62	HGBR2	436	J 6/62	LI2
376	J 6/62	HGO(S)	437	J 6/62	LI2CL2
377	J 6/74	I	438	J12/68	LI2F2
378	J 9/61	I2(S)	439	J 3/64	LI2O(S)
379	J 9/61	I2(L)	440	J 3/64	LI2O(L)
380	J 9/61	I2	441	J 3/64	LI2O
381	J12/61	K(S)	442	J 3/64	LI2O2
382	J12/61	K(L)	443	J 6/71	LI2O2H2
383	J 6/62	K	444	J 6/62	LI3CL3
384	J 3/65	K+	445	J12/68	LI3F3
385	J 6/71	KBO2	446	J 9/62	MG(S)
386	J 3/66	KCL(S)	447	J 9/62	MG(L)
387	J 3/66	KCL(L)	448	J 9/62	MG
388	J 3/66	KCL	449	J12/70	MG+
389	J 6/69	KF(S)	450	J 6/75	MGBR
390	J 6/69	KF(L)	451	J 6/74	MGBR2(S)
391	J 6/69	KF	452	J 6/74	MGBR2(L)
392	J12/68	KF2-	453	J 6/74	MGBR2
393	J 6/71	KHF2(S)	454	J12/66	MGCO3(S)
394	J 6/71	KHF2(S)	455	J 3/66	MGCL
395	J 6/71	KHF2(L)	456	J 6/68	MGCL+
396	J12/67	KO	457	J 3/66	MGCLF
397	J12/67	KO-	458	J12/65	MGCL2(S)
398	J12/70	KOH	459	J12/65	MGCL2(L)
399	J12/70	KOH(S)	460	J12/69	MGCL2
400	J12/70	KOH(S)	461	J12/75	MGF
401	J12/70	KOH(L)	462	J12/75	MGF+
402	J12/71	KOH+	463	J 6/75	MGF2(S)
403	J12/61	K2	464	J 6/75	MGF2(L)
404	J 3/66	K2CO3(S)	465	J 6/75	MGF2
405	J 3/66	K2CO3(L)	466	J12/75	MGF2+
406	J 6/69	K2F2	467	J12/66	MGH
407	J 6/63	K2O(S)	468	J12/74	MGI
408	J12/70	K2O2H2	469	J12/74	MGI2(S)
409	J12/71	K2SO4(S)	470	J12/74	MGI2(L)
410	J12/71	K2SO4(S)	471	J12/74	MGI2
411	J12/71	K2SO4(L)	472	J 3/64	MGN
412	J 6/62	LI(S)	473	J12/74	MGO(S)
413	J 6/62	LI(L)	474	J12/74	MGO(L)
414	J 6/62	LI	475	J12/74	MGO
415	J 3/65	LI+	476	J12/75	MGOH
416	J 6/71	LIBO2	477	J12/75	MGOH+
417	J 6/62	LICL(S)	478	J12/75	MGO2H2(S)
418	J 6/62	LICL(L)	479	J12/75	MGO2H2
419	J 6/62	LICL	480	J12/71	MGS(S)
420	J12/68	LIF(S)	481	J 6/71	MGS
421	J12/68	LIF(L)	482	L 7/76	MGSO4(S)
422	J12/68	LIF	483	L 7/76	MGSO4(L)
423	J12/68	LIF2-	484	J12/67	MGSIO3(S)
424	J 9/65	LIFO	485	J12/67	MGSIO3(S)
425	J 9/67	LIH(S)	486	J12/67	MGSIO3(S)
426	J 9/67	LIH(L)	487	J12/67	MGSIO3(L)
427	J 9/67	LIH	488	J12/75	MG2F4

Figure 4.3-11 (continued): list of the JANNAF.THE species.

489	J12/67	MG2SIO4(S)	550	J12/64	NA2CL2
490	J12/67	MG2SIO4(L)	551	J12/68	NA2F2
491	J 3/61	N	552	J 6/68	NA2O(S)
492	J12/70	NCO	553	J 6/68	NA2O(S)
493	J 6/65	NF	554	J 6/68	NA2O(L)
494	J 3/64	NF2	555	K10/74	NA2O
495	J 6/69	NF3	556	J12/70	NA2O2H2
496	J12/71	NH	557	J12/66	NA2SO4(S)
497	J12/65	NH2	558	J12/66	NA2SO4(S)
498	J 9/65	NH3	559	J12/66	NA2SO4(S)
499	J 6/63	NO	560	J12/66	NA2SO4(L)
500	J 6/66	NO+	561	K11/74	NA2SO4
501	J12/72	NOCL	562	J12/73	NB(S)
502	J 6/61	NOF	563	J12/73	NB(L)
503	J 6/70	NOF3	564	J12/73	NB
504	J 9/64	NO2	565	J12/73	NBO(S)
505	J 6/72	NO2-	566	J12/73	NBO(L)
506	J12/65	NO2CL	567	J12/73	NBO
507	J12/65	NO2F	568	J12/73	NBO2(S)
508	J12/64	NO3	569	J12/73	NBO2(L)
509	J 6/61	NZR(S)	570	J12/73	NBO2
510	J 6/61	NZR(L)	571	J12/72	NB2O5(S)
511	J 6/63	NZR	572	J12/72	NB2O5(L)
512	J 9/65	N2	573	L 5/66	NE
513	J12/65	N2H4	574	L12/66	NE+
514	J12/64	N2O	575	J 6/74	O
515	J12/70	N2O+	576	L12/66	O+
516	J 9/64	N2O4	577	J 6/65	O-
517	J12/64	N2O5	578	J12/70	OH
518	J12/70	N3	579	J12/70	OH+
519	J 6/62	NA(S)	580	J12/70	OH-
520	J 6/62	NA(L)	581	J12/65	OZR
521	J 6/62	NA	582	J 9/65	O2
522	J 3/65	NA+	583	J12/66	O2-
523	J 6/71	NABO2	584	J12/65	O2ZR(S)
524	J 9/64	NABR(S)	585	J12/65	O2ZR(S)
525	J 9/64	NABR(L)	586	J12/65	O2ZR(L)
526	J 9/64	NABR	587	J12/65	O2ZR
527	J3/66	NACN	588	J 6/61	O3
528	J 9/64	NACL(S)	589	J 6/62	P
529	J 9/64	NACL(L)	590	J 6/61	P(S)
530	J12/64	NACL	591	L12/66	P+
531	J12/68	NAF(S)	592	J 6/70	PCL3
532	J12/68	NAF(L)	593	J12/69	PF3
533	J12/68	NAF	594	J12/69	PF5
534	J12/68	NAF2-	595	J 6/67	PH
535	J 3/63	NAH	596	J 6/62	PH3
536	J 9/63	NAI(S)	597	J 9/62	PN
537	J 9/63	NAI(L)	598	J 6/71	PO
538	L 6/72	NAI	599	J 6/67	PS
539	J12/67	NAO	600	J 6/61	P2
540	J12/67	NAO-	601	J 6/61	P4
541	J12/70	NAOH(S)	602	J 3/62	PB(S)
542	J12/70	NAOH(L)	603	J 3/62	PB(L)
543	J12/70	NAOH	604	J 3/62	PB
544	J12/71	NAOH+	605	J12/73	PBBR
545	J 6/62	NA2	606	J12/73	PBBR2(S)
546	J 3/66	NA2CO3(S)	607	J12/73	PBBR2(L)
547	J 3/66	NA2CO3(S)	608	J12/73	PBBR2
548	J 3/66	NA2CO3(L)	609	J12/73	PBBR4
549	J3/66	NA2C2N2	610	J 6/73	PBCL

Figure 4.3-12 (continued): list of the JANNAF.THE species.

611	J 6/73	PBCL+	672	J 9/67	SIO2
612	J 6/73	PBCL2(S)	673	J12/71	SIS
613	J 6/73	PBCL2(L)	674	J 3/67	SI2
614	J 6/73	PBCL2	675	J 3/67	SI2C
615	J 6/73	PBCL2+	676	J 3/67	SI2N
616	J12/73	PBCL4	677	J 3/67	SI3
617	J12/73	PBF	678	J12/70	SR(S)
618	J12/73	PBF2(S)	679	J12/70	SR(L)
619	J12/73	PBF2(S)	680	J12/70	SR
620	J12/73	PBF2(L)	681	J12/74	SRBR
621	J12/73	PBF2	682	J12/72	SRCL
622	J12/73	PBF4	683	J12/72	SRCL2(S)
623	J12/73	PBI	684	J12/72	SRCL2(S)
624	J12/73	PBI2(S)	685	J12/72	SRCL2(L)
625	J12/73	PBI2(L)	686	J12/72	SRCL2
626	J12/73	PBI2	687	J12/72	SRF
627	J12/73	PBI4	688	J12/72	SRF+
628	J 6/73	PBS(S)	689	J12/72	SRF2(S)
629	J 6/73	PBS(L)	690	J12/72	SRF2(L)
630	J 6/73	PBS	691	J12/72	SRF2
631	J 9/63	PB2	692	J 6/74	SRI2
632	J12/65	S(S)	693	J12/72	SRO(S)
633	J12/65	S(L)	694	J12/72	SRO(L)
634	J 6/71	S	695	J 6/74	SRO
635	L12/66	S+	696	J12/75	SROH
636	J12/69	SF4	697	J12/75	SRO2H2(S)
637	J 9/65	SF6	698	J12/75	SRO2H2(L)
638	J 6/67	SH	699	J12/75	SRO2H2
639	J 6/61	SN	700	J12/72	TA(S)
640	J 6/71	SO	701	J12/72	TA(L)
641	J 6/72	SOF2	702	J12/72	TA
642	J 6/61	SO2	703	J12/73	TAC(S)
643	J 6/71	SO2CL2	704	J12/73	TAC(L)
644	J 6/71	SO2CLF	705	J12/73	TAO
645	J 6/71	SO2F2	706	J12/73	TAO2
646	J 9/65	SO3	707	J12/72	TA2O5(S)
647	J12/65	S2	708	J12/72	TA2O5(L)
648	J6/64	S8	709	J 6/73	V(S)
649	J 3/67	SI(S)	710	J 6/73	V(L)
650	J 3/67	SI(L)	711	J 6/73	V
651	J 3/67	SI	712	L 2/76	VCL2(S)
652	J12/71	SI+	713	L 2/76	VCL3(S)
653	J 3/67	SIC	714	L 2/76	VCL4(L)
654	J 3/67	SIC2	715	L 2/76	VCL4
655	J 9/67	SICL	716	J12/73	VN(S)
656	J12/70	SICL2	717	J12/73	VN
657	J12/69	SICL3	718	J12/73	VO(S)
658	J12/70	SICL4	719	J12/73	VO(L)
659	J12/69	SIF	720	J12/73	VO
660	J12/68	SIF2	721	J12/73	VO2
661	J 6/70	SIF3	722	J12/73	V2O3(S)
662	J 9/63	SIF4	723	J12/73	V2O3(L)
663	J12/69	SIH	724	J 6/73	V2O4(S)
664	J12/71	SIH+	725	J12/73	V2O4(S)
665	J12/60	SIH4	726	J 6/73	V2O4(L)
666	J 3/67	SIN	727	J 6/73	V2O5(S)
667	J 9/67	SIO	728	J 6/73	V2O5(L)
668	J 6/67	SIO2(S)	729	L 4/70	XE
669	J 6/67	SIO2(S)	730	J12/67	ZR(S)
670	J 6/67	SIO2(S)	731	J12/67	ZR(S)
671	J 6/67	SIO2(L)	732	J12/67	ZR(L)
			733	J 6/61	ZR

Figure 4.3-13 (continued): list of the JANNAF.THE species.

5 THEORETICAL ANALYSIS

5.1 SCIENTIFIC SOURCE-REFERENCE

Several computation developments of chemical equilibrium compositions were made at the NASA Lewis Research Center, [RD2] resulting to a software named CEC 71 (Chemical Equilibrium Calculations 1971). The ODE program, which is set out in this report, is an adaptation of this program to the computation of the plume effects.

This version using the knowledge from 1965 to 1967, calculates the chemical compositions of the system, with a free-energy minimization technique.

5.2 BASIC METHODS

When several chemical species are brought together, chemical reactions occur, during which species disappear or appear. After a while, the concentrations of various species no longer change : the chemical equilibrium is established. The computation of the equilibrium concentrations is the main function of ODE.

- for a set of given species, the chemical equilibrium depends on the thermodynamic state of the system ; this state may be specified by assigning two independent thermodynamic state functions, which can be for a thruster (open system) :
  - pressure and temperature (P, T),
  - pressure and enthalpy (P, H),
  - pressure and entropy (P, S).
- for an assigned thermodynamic state, it is shown that the equilibrium concentrations correspond to a minimum free-energy. The generalized method of solution used in ODE is based on the free-energy minimization, with the following constraints.
  - atom conservation,
  - assigned thermodynamic state.

The equations associated with these definitions are :

Gibbs free-energy :

$$G = H - TS$$

with : H : enthalpy per kg of mixture.

S : entropy per kg of mixture.

T : temperature of the mixture.

For a mixture of N species, the Gibbs free-energy per kg of mixture is given by :

$$G = \sum_{j=1}^{N} n_j \mu_j$$

where μ_j is the chemical potential per kmole of species j,

n_j is the number of kmole of species j per kg of mixture.

μ_j is defined by $G = \sum_{j=1}^{N} n_j \mu_j$ for gaseous phase,

$\mu_j = \mu_j^0$ for condensed phase.

where : μ_j^0 is the standard state chemical potential for species j under one atmosphere, according to T.

P, T are the pressure and the temperature defining the thermodynamic state.

n is the total number of kmole per kg of mixture :

$$n = \sum_{j=1}^{N} n_j$$

The atom conservation is expressed by the relationship :

$$b_i = \sum_{j=1}^{N} a_{ij} n_j = b_i^0 \quad \text{for i=1,..., L}$$

where : L is the number of different elements in the initial reactants.

b_i is the number of katoms of element i per kg of mixture (initial reactants).

a_{ij} is the stoichiometric coefficients (katoms of element i per kmole of species j).

The mixture thermodynamic functions are given by :

$$H(T) = \sum_{j=1}^{N} n_j H_j^0(T) \qquad \text{(in J/kg)}$$

$$S(T) = \sum_{j=1}^{N} n_j S_j^0(T) - R \log P \qquad \text{(in J/kg/K)}$$

For each species j, the functions $H_j^0(T)$ and $S_j^0(T)$ are tabulated in the file JANNAF.THE.

The method of free-energy minimization is based on a Newton iterative resolution ; the quantity to be minimized is a combination of the free-energy and the atom conservation equation :

$$F = G + \sum_{i=1}^{L} \lambda_i (b_i - b_i^0)$$

where λ_i is a Lagrange multiplier.

The initial conditions are :

- for the first computation (chamber) : the n_j have the same value.
- for the other computations (expansion) : the n_j values are those from the previous computations.

According to the cases, ODE solves 3 types of problems :

- in the chamber : P and T are given :
  - minimization of F then computation of n_j.
  - computation of H and S.
- in the chamber : P and H are known :
  - minimization of F then computation of n_j and T.
  - computation of S.
- isentropic expansion : P is given, S = S (chamber) :
  - minimization of F then computation of n_j and T.
  - computation of H and V (gas velocity).

5.3 TABULATION OF GASEOUS MIXTURE PROPERTIES

In the following equations, subscript 0 corresponds to the chamber values, which are supposed to be already computed.

The gaseous mixture is assumed to be <u>frozen</u> :

$$S = S_0$$

$$N_j = nj_0$$

T is computed from the entropy equation :

$$S_0 = \sum_j n_j S_j^0(T) - R \log P$$

The other values are computed with :

$$x_j = \frac{n_j}{\sum_j n_j} \qquad \text{molar fraction of species j.}$$

$$M_w = \sum_j x_j M_{wj} \qquad \text{molar weight in kg/kmole.}$$

$$H(T) = \sum_j x_j H_j(T) \qquad \text{enthalpy in J/kg.}$$

$$Cp(T) = \sum_j x_j Cp_j(T) \qquad \text{specific heat in J/kg/K.}$$

$$R = \frac{8314}{M_w} \qquad \text{gas constant.}$$

$$\gamma = \frac{Cp}{Cp - R} \qquad \text{specific heat ratio.}$$

$$V = \sqrt{2(H_0 - H)} \qquad \text{gas velocity.}$$

The viscosity μ and the thermal conductivity coefficient k of the mixture are computed from μ and k coefficients of each species, by semi-empirical mixture-correlations due to Wilke.

The Prandtl number is given by :

$$\mathrm{Pr} = \frac{\mu Cp}{k}$$

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