Continuum, Inc.

SUITE 102
4717 UNIVERSITY DRIVE
Huntsville, Alabama 358
(205) 837-9310

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An Investigation of Equilibrium Concepts

Final Report

Prepared for
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by R. J. Prozan

FOREWORD and SUMMARY

This document is the final report to the National Aeronautics and Space Administration, George C. Marshall Space Flight Center, Marshall Space Flight Center, Huntsville , Alabama. This effort was performed by Continuum, Inc., Huntsville, Alabama under Contract Number NAS 8-34946. The technical representative from MSFC was Mr. Klaus Gross.

The information presented here deals with a different approach to modelling of the thermochemistry of rocket engine combustion phenomena. While the approach is essentially unverified by extensive test data, it does advance a rationale that explains some troubling discepancies in the conventional model. The methodology described here is based on the Continuum, Inc. hypothesis of a new variational principle applicable to compressible fluid mechanics. This hypothesis is extended to treat the thermochemical behavior of a reacting (equilibrium) gas in an open system.

NOMENCLATURE

The nomenclature used in this report is consistent with that given in reference (2) with the following additions;

Φ_α	forcing function modifying the Gibbs function
λ^E	defined in text
Ω_1, Ω_2	defined in text
η	defined in text

INTRODUCTION

This study deals with the determination of chemical equilibrium in steady flowing systems subject to downstream boundary conditions. Research at Continuum, Inc. has recently lead to the hypothesis of a new variational principle for compressible fluid mechanics. This principle , which has permitted impressive advances in numerical computations of unsteady flows, is extended to treat the one dimensional combustion and expansion of reacting gases in rocket engines.

The study of the flow of reacting gases has perhaps its most important application in rocket engines for use in the aerospace field. The performance of an engine in these applications is a critical consideration. For this reason precise methods are needed to predict, in a preliminary design, the thrust and mass flow of a proposed engine. Unfortunately this performance evaluation is extremely complex. Many imperfectly understood phenomena combine to create the combustion process while the ensuing hostile environment makes experimental measurements of all but gross quantities virtually impossible.

The concept of equilibrium chemical reactions is invaluable in the performance evaluation of rocket engines. Although all reactions in a real engine progress at a finite rate, the assumption of equilibrium (infinite rates) provides meaningful information with a comparatively simple calculation. The equilibrium methodology is well acccepted but, because of its importance, a reexamination of the concepts is justifiable.

Another reason for concern is that, after all effects such as droplet vaporization, reaction kinetics, fuel striations, divergence losses, boundary layer losses, etc. are accounted for, unacceptable errors may still exist in the performance evaluation. This discrepancy has been termed a combustion efficiency problem. The explanation usually given is that some of the above mechanisms may be imperfectly understood and that not enough experimental data has been gathered to adequately define some of the required parameters. Although this argument has merit and is certainly correct to some degree, other phenomena which would account for the errors are possible.

Several factors influenced the decision to pursue the questioning of equilibrium concepts. Performance calculations based conventional equilibrium concepts seemed to give systematically erroneous results. The adiabatic flame and isentropic expansion solution, typified by Zeleznick and Gordon (1) gave good mass flows but overpredicted thrust and, therefore, specific impulse.

Now the adiabatic flame calculation assumes an infinite area duct at the combustion front. Real engines, of course, posses a finite area duct and it is well known that combustion in such a duct causes a total pressure drop. This effect is discussed in many texts using simple heating relations. Consideration of this effect in rocket performance analyses served to reduce the thrust to approximately the right value but had the disconcerting effect of reducing the mass flow rate proportionately such that the impulse remained in error.

The chemical equilibrium calculation itself had never been questioned. Proceeding from the premise that the effects were related and the apparent discrepancy of mass, thrust and impulse showed up in even the most basic building block (the equilibrium analysis) of the performance evaluation, it was postulated by Prozan (2) that the throat choking condition acts as a constraint to the combustion process. That study was not well received and the matter remained unquestioned and unresolved for many years.

Recently, however, research at Continuum led to the hypothesis of a variational principle for compressible flow. Prozan (3,4) advanced the following statements for consideration as the long sought after variational principle governing fluid mechanics;

I. For the maximum stability of any real system, which may or may not be isolated from a larger universe, the rate of production of extensive entropy is a maximum subject to the constraints upon its' formation.

II. For the equilibrium or time invariant state of such a system, the extensive entropy production must be a maximum subject to the constraints upon its formation. Consequently the entropy delivered to the universe, should the system not be isolated, must also be a maximum.

The first statement has been successfully used in unsteady flow of a compressible ideal gas to produce a numerical analog which is absolutely conservative and stable. The hypothesis, then, has been supported in at least one branch of fluid mechanics. Since the original study of reference (2) is based on the same general principle, it seemed possible, even probable, that the thermochemical behavior of flowing systems was related to the hypothesized principle. Now the second statement is a consequence of the first statement for steady state. It states that the delivery of extensive entropy to the universe is a maximum for an open system.

It is useful at this juncture to review the premise upon which conventional thermochemistry calculation are based. The statements of Gibbs (5) provide the foundation for the analysis of reference (1) and similiar calculations. The classical Gibbs statements are;

I. "For the equilibrium of any isolated system it is necessary and sufficient that in all possible variations of the state which do not alter its energy, the variation of its entropy shall vanish or be negative."

II. "For the equilibrium of any isolated system it is necesssary and sufficient that in all possible vaiations in the state of the system which do not alter its entropy, the variation of its energy shall either vanish or be negative."

The author has no argument with the Gibbs statements. The point of contention is the interpretation of these statements and their application to thermochemical calculations in open systems. First notice that Gibbs statements deal with isolated systems. Gibbs therefore dealt with thermostatics but not necessarily with thermodynamics. Secondly the Gibbs statements do refer to all possible variations in the state. It is the contention of this study that any final solution value which does not satisfy the throat condition is not a possible state.

A final point which should be mentioned before proceeding with the discussion relates to the formation of the Gibbs functional. The previous two statements by Gibbs and the assumption of constant temperature and pressure permit one to develop the point thermodynamic function known as Gibbs free energy. It is this free energy function which is used in conventional thermodynamic calculations. The consequences of considering constant temperature and pressure in a changing pressure, temperature situation need to be addressed.

The following technical discussion closely follows the previous study found in reference (2). The equilibrium combustion constrained by an ideal gas expansion to the throat is duplicated from that reference. In addition an equilibrium expansion from chamber to throat is included. In the interest of brevity the salient features of that reference will not be repeated, but alterations and expansions upon that study will be discussed. Whereever possible, the same nomenclature and units are used.

TECHNICAL DISCUSSION

Ideal Expansion from Chamber to Throat

The procedure found in reference (2) is followed exactly in this study with the exception that the first two equations found in equation set (23) of that report were solved analytically rather than numerically for λ^M and λ^T . This led to a final set of equations to solve which are much simpler than those shown in the reference. This new set follows;

$$g_\alpha + \sum^{n} \lambda_j a_{j\alpha} + \Phi_\alpha = 0 \qquad (\alpha = 1,m)$$

$$\sum^{m} a_{j\alpha}\mu_\alpha - N_j = 0 \qquad (j = 1,n)$$

$$p + b_1\nu = \bar{p}_{inj}$$

$$h + \frac{b_2}{2}\nu^2 = h_0$$

$$\ln (A^*/A_T) = 0$$

where $\Phi_\alpha = \bar{\lambda}^E(h_\alpha/T - \psi \frac{\partial h}{\partial T})$

and where $\bar{\lambda}^E = \lambda^E T - 1$

Note that the system of equations has been cast so that it looks like the normal Gibbs function treatment except for the throat constraint and the new forcing function Φ_α . The results were in substantial agreement with the reference (differing slightly because different thermodynamic parameters are available today).

Equilibrium Expansion from Chamber to Throat

In the equilibrium expansion from the chamber to the throat, the same optimization function was used. That is, the entropy was maximized subject to the system constraints. In this treatment, however, instead of varying a Lagrange multiplier to satisfy the throat constraint, the number of moles of the species OH was used to satify the throat constraint. This is actually the amount of OH at the throat rather than the amount of post combustion OH. Proceeding in the same fashion as the reference the entropy maximization statement was constrained by momentum and energy and the throat choking condition. The other difference between the equilibrium expansion and the ideal gas expansion comes from the integration of the equations of motion during the expansion rather than the previous ideal treatment. For each station during the expansion or integration the entropy is maximized subject to the momentum and energy constraints locally. The system of equations used to describe the process is the same as those shown earlier except that;

$$\bar{\lambda}^E = (b_2 \nu^2 \Omega_1 - C_2 T \Omega_2/\psi)/(T\frac{\partial h}{\partial T} + b_2 \nu^2 \Omega_1)$$

where $\Omega_1 = p\eta/(p\eta - b_1 \nu)$ and $\Omega_2 = b_1 \nu/(p\eta - b_1 \nu)$ where $\eta = \frac{(A^{k-1} + A^k)}{2 A^k}$

In the solution procedure the chamber solution is made by setting A^{k-1} and A^k (denoting area of the previous station and the current station respectively) to the combustor area. The number of moles of OH is held fixed. The integration is then performed from chamber to throat by decreasing the pressure slightly from station to station. The crossectional area is found from the momentum equation for this new pressure.

It was very interesting to note that the expansion was isentropic even though the entropy was being maximized. This was what was expected, but attaining an isentropic expansion with this procedure was never the less encouraging. The seemingly contradictory result can be interpreted in the following fashion.

The variational principle states that the entropy delivered to the universe must be a maximum. This must be the case even during an isentropic expansion. The locus of states that represents equilibrium is a series of maximum values of entropy whose value during the expansion is constant. This concept is not really hard to understand since, if the entropy is truly a maximum, then during a slow and continuous expansion it should stay constant or isentropic. The principle, if correct, should predict this behavior. No success has resulted from a limited attempt to apply the principle beyond the throat. To solve this problem was beyond the scope of work of the contract and beyond the available funds in the contract.

A computer program has been written to perform the calculations of equilibrium combustion and equilibrium orideal expansion between combustor and throat. This program is included in this report as an Appendix. Hopefully the calculations are sufficiently well anotated that the program is easily understood.
Where ever possible common terminology is used between report and program.

Conclusions

The entire subject is of great importance and certainly is of great academic interest. The concepts appear to have potential to explain some of the propulsion prediction discrepancies but are essentially unverified. The issue is best resolved by a dedicated test program which attempts to experimentally provide data for cases in which the constrained theory will predict a large difference from the conventional approach.

Before such a test program be conducted, however, the analysis should be extended into the supersonic regime of the nozzle. A successful solution of supersonic expansion would then allow one to more accurately assess the performance alterations caused by the new modelling concept.

REFERENCES

1. Zeleznik, R. J., and S. Gordon, "A General IBM 704 or 7090 Computer Program for Computation of Chemical Equilibrium Compositions, Rocket Performance, and Chapman-Jouguet Detonations, "NASA TN D-1454, October 1962.

2. Prozan, R. J.,"Maximization of Entropy for Equilibrium Processes with Emphasis on Rocket Engine Combustion Phenomena",LMSC/HREC D149342, October 1969.

3. Prozan, R. J.,"A Variational Principle for Compressible Fluid Mechanics(Discussion of the One-Dimensional Theory)", NASA CR 3526, April 1982.

4. Prozan, R. J.,"A Variational Principle for Compressible Fluid Mechanics(Discussion of the Multi-Dimensional Theory), NASA CR (in publication).

5. Gibbs, J. W.,"On the Equilibrium of Heterogeneous Substances - Gibbs Collected Works, Yale University Press, New Haven, Conn., 1928.

APPENDIX

```
  100 CALL HASA
      ICNST=7
C     COMPUTE FORCING FUNCTION TO ALTER GIBBS FUNCTION
      DO 110 I=1,6
      PHI(I)=ALAME*(HA(I)-T*W*DHDT)
  110 CONTINUE
C     FIND NEW EQUILIBRIUM POSITION FOR THIS P,T
      CALL EQUIL(ICNST)
C     SOLVE MOMENTUM AND ENERGY EQUATIONS FOR NEW P,T
      CALL HASA
      BM=C3*C1/(AC*AC)
      BE=C4*C1*C1/(AC*AC)
      P=.5*PF+SQRT(.25*PF*PF-BM*T/W)
      ENU=T/(P*W)
      HERR=H+.5*BE*ENU*ENU-HF
C     DRIVE ENERGY ERROR TO ZERO
      CALL ITSUB(T,HERR,20,.1,SAVEIT)
      IBR=IFIX(SAVEIT(1))
      GOTO (100,100,100,100,200,200),IBR
  200 CONTINUE
C     SOLUTION OF ALL EQUATIONS EXCEPT THE THROAT CONSTRAINT HAS
C     CONVERGED FOR THIS VALUE OF ALAME
      EM=SQRT(BM*T/(W*GAMMA))/P
      TFOT=1.+.5*(GAMMA-1.)*EM*EM
C     FIND THE CHOKING AREA FOR THIS ALAME
      ASOACL=ATDET(GAMMA,EM,ASTAR)
      ASOATL=ASOACL+ALOG(AC/AT)
C     CHANGE ALAME TO DRIVE LOG(ASTAR/AT) TO ZERO
      CALL ITSUB(ALAME,ASOATL,20,.0001,SAVEIL)
      IBR=IFIX(SAVEIL(1))
      GOTO (20,20,20,20,300,300),IBR
  300 CONTINUE
C     SOLUTION HAS CONVERGED - PRINT COMBUSTOR AND THROAT RESULTS
      RHO=P*W/(C1*T)
      VEL=1./(RHO*AC)
      WRITE(6,9930)
      WRITE(6,9800)
      WRITE(6,9810) T,P,RHO,EM,VEL
      WRITE(6,9840) W
      WRITE(6,9410)
      WRITE(6,9820) (XA(I),I=1,6)
      WRITE(6,9830) (EMUA(I),I=1,6)
      WRITE(6,9100)
      TS=T*TFOT/(.5*(GAMMA+1.))
      PS=P*((TS/T)**(GAMMA/(GAMMA-1.)))
      RHOS=PS*W/(C1*TS)
      VELS=1./(RHOS*AT)
      AISPS=(PS*AT+C3*VELS)/(9.807*C3)
      WRITE(6,9900)
      WRITE(6,9910) AISPS,TS,PS,RHOS,VELS
      WRITE(6,9100)
C
C     ENTER THE CALCULATION OF THE EQUILIBRIUM EXPANSION TO THE THROAT
C
```

```
  100 CALL HASA
      ICNST=7
C     COMPUTE FORCING FUNCTION TO ALTER GIBBS FUNCTION
      DO 110 I=1,6
      PHI(I)=ALAME*(HA(I)-T*W*DHDT)
  110 CONTINUE
C     FIND NEW EQUILIBRIUM POSITION FOR THIS P,T
      CALL EQUIL(ICNST)
C     SOLVE MOMENTUM AND ENERGY EQUATIONS FOR NEW P,T
      CALL HASA
      BM=C3*C1/(AC*AC)
      BE=C4*C1*C1/(AC*AC)
      P=.5*PF+SQRT(.25*PF*PF-BM*T/W)
      ENU=T/(P*W)
      HERR=H+.5*BE*ENU*ENU-HF
C     DRIVE ENERGY ERROR TO ZERO
      CALL ITSUB(T,HERR,20,.1,SAVEIT)
      IBR=IFIX(SAVEIT(1))
      GOTO (100,100,100,100,200,200),IBR
  200 CONTINUE
C     SOLUTION OF ALL EQUATIONS EXCEPT THE THROAT CONSTRAINT HAS
C     CONVERGED FOR THIS VALUE OF ALAME
      EM=SQRT(BM*T/(W*GAMMA))/P
      TFOT=1.+.5*(GAMMA-1.)*EM*EM
C     FIND THE CHOKING AREA FOR THIS ALAME
      ASOACL=ATDET(GAMMA,EM,ASTAR)
      ASOATL=ASOACL+ALOG(AC/AT)
C     CHANGE ALAME TO DRIVE LOG(ASTAR/AT) TO ZERO
      CALL ITSUB(ALAME,ASOATL,20,.0001,SAVEIL)
      IBR=IFIX(SAVEIL(1))
      GOTO (20,20,20,20,300,300),IBR
  300 CONTINUE
C     SOLUTION HAS CONVERGED - PRINT COMBUSTOR AND THROAT RESULTS
      RHO=P*W/(C1*T)
      VEL=1./(RHO*AC)
      WRITE(6,9930)
      WRITE(6,9800)
      WRITE(6,9810) T,P,RHO,EM,VEL
      WRITE(6,9840) W
      WRITE(6,9410)
      WRITE(6,9820) (XA(I),I=1,6)
      WRITE(6,9830) (EMUA(I),I=1,6)
      WRITE(6,9100)
      TS=T*TFOT/(.5*(GAMMA+1.))
      PS=P*((TS/T)**(GAMMA/(GAMMA-1.)))
      RHOS=PS*W/(C1*TS)
      VELS=1./(RHOS*AT)
      AISPS=(PS*AT+C3*VELS)/(9.807*C3)
      WRITE(6,9900)
      WRITE(6,9910) AISPS,TS,PS,RHOS,VELS
      WRITE(6,9100)
C
C     ENTER THE CALCULATION OF THE EQUILIBRIUM EXPANSION TO THE THROAT
C
```

```
C     SAVE IDEAL SOLUTION FOR INITIAL GUESS
 1000 GAMMAC=GAMMA
      TC=T
      PC=P
      FC=PF*AC
      WC=W
      RHOC=RHO
C     INITIALIZE LOOP IN WHICH EMU(OH) WILL BE VARIED TO SATISFY THE THROAT
C     CONSTRAINT
      SAVEIL(1)=1.
      SAVEIL(2)=-.4*EMUA(5)
      LOOP4=0
      DO 1010 I=1,6
      EMUAC(I)=EMUA(I)
 1010 CONTINUE
 1020 DO 1030 I=1,6
      EMUA(I)=EMUAC(I)
 1030 CONTINUE
      ANM1=AC
      GAMMA=GAMMAC
      FNM1=FC
      RHONM1=RHOC
      PNM1=P
      W=WC
      AN=AC
      T=TC
      P=PC
C     DELTA MAY BE CHANGED TO MAKE SOLUTION MORE OR LESS ACCURATE
      DELTA=.01
      LOOP3=0
C     REDUCE P FOR EXPANSION - NOTE THAT THIS IS IGNORED FOR FIRST PASS
 1100 P=P*(1.-DELTA)
 1110 IF (LOOP3.EQ.0) GOTO 1120
      QA=.5*(P-PNM1)
      QB=.5*(P+PNM1)*ANM1-FNM1
      QC=C3*C1*T/(P*W)
C     COMPUTE THE DUCT AREA THAT WILL SATISFY THE MOMENTUM EQUATION
C     KNOWINC THE PRESSURE - IGNORE ON FIRST PASS
      AN=.5*(-QB-SQRT(QB*QB-4.*QA*QC))/QA
      GOTO 1130
 1120 QB=FNM1/AC
      QA=1.
      QC=C3*C1*T/(AC*AC*W)
C     COMPUTE THE PRESSURE THAT WILL SATISFY MOMENTUM KNOWING AREA
C     FIRST PASS ONLY
      P=.5*(QB+SQRT(QB*QB-4.*QA*QC))
C     COMPUTE FORCING FUNCTION
 1130 BE=C4*C1*C1/(AN*AN)
      BM=C3*C1/(AN*AN)
      ARAT=.5*(ANM1+AN)/AN
      ENU=T/(P*W)
      BMENU=BM*ENU
      OP=BMENU/(P*ARAT-BMENU)
      PP1OP=P*ARAT/(P*ARAT-BMENU)
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C      GET NEW THERMO PROPERTIES
       CALL HASA
       XNUM1=BE*ENU*ENU*PP1OP-C2*T*OP/W
       XNUM2=T*DHDT+BE*ENU*ENU*PP1OP
       ALAME=-XNUM1/XNUM2
       DO 1140 I=1,6
       PHI(I)=ALAME*(HA(I)/T-W*DHDT)
 1140  CONTINUE
       ICNST=5
C      GET NEW EQUILIBRIUM SOLUTION FOR THIS DUCT POSITION WHILE HOLDING
C      EMUA(OH) CONSTANT
       CALL EQUIL(ICNST)
       CALL HASA
       ENU=T/(P*W)
       DHFDT=-DHDT-BE*ENU*ENU/T
       DHF=HF-H-.5*BE*ENU*ENU
       T=T-.5*DHF/DHFDT
C      DRIVE ENERGY ERROR TO ZERO
       IF (ABS(DHF).GT.DELTA) GOTO 1110
C      COMBUSTOR SOLUTION FOR THIS MOLE FRACTION VALUE HAS CONVERGED
       RHO=P*W/(C1*T)
       VEL=1./(RHO*AN)
       DLOGP=2.*(PNM1-P)/(PNM1+P)
       DLOGR=2.*(RHONM1-RHO)/(RHONM1+RHO)
       IF (LOOP3.GT.0) GAMMA=DLOGP/DLOGR
       EM=SQRT(BM*T/(GAMMA*W))/P
       IF (LOOP3.GT.0) GOTO 1160
C      SAVE CHAMBER RESULTS
       SC=S
       TC=T
       PC=P
       WC=W
       RHOC=RHO
       EMC=EM
       VELC=VEL
       DO 1150 I=1,6
       EMUAC(I)=EMUA(I)
 1150  CONTINUE
 1160  LOOP3=LOOP3+1
       RHONM1=RHO
       ANM1=AN
       PNM1=P
       FNM1=(P+BM*ENU)*AN
       ASOANL=ATDET(GAMMA,EM,ASOAN)
C      SINCE THROAT IS A SINGULARITY FOR THIS FORMULATION GET THE PROPER
C      AREA WITHIN 1 PER CENT AND USE IDEAL GAS EXTRAPOLATION BEYOND THAT
C      IF NOT WITHIN TOLERANCE GO BACK AND REDUCE PRESSURE
       IF (ABS(ASOANL).GT..01) GOTO 1100
       ASTAR=ASOAN*AN
       AOATL=ASOANL+ALOG(AN/AT)
C      ALTER AMOUNT OF OH WHICH WILL BE PRESENT TO SATISFY THROAT
       CALL ITSUB(EMUAC(5),AOATL,20,.001,SAVEIL)
       IBR=IFIX(SAVEIL(1))
       GOTO (1020,1020,1020,1020,1200,1200),IBR
```

```
C     SOLUTION HAS CONVERGED . PRINT RESULTS
1200  WRITE(6,9920)
      WRITE(6,9800)
      WRITE(6,9810) TC,PC,RHOC,EMC,VELC
      WRITE(6,9840) WC
      WRITE(6,9410)
      DO 1210 I=1,6
      XA(I)=WC*EMUAC(I)
 1210 CONTINUE
      WRITE(6,9820) (XA(I),I=1,6)
      WRITE(6,9830) (EMUAC(I),I=1,6)
      WRITE(6,9100)
      DO 1220 I=1.6
      XA(I)=W*EMUA(I)
 1220 CONTINUE
      TS=T*(1.+.5*(GAMMA-1.)*EM*EM)/(.5*(GAMMA+1.))
      PS=P*((TS/T)**(GAMMA/(GAMMA-1.)))
      RHOS=PS*W/(C1*TS)
      VELS=1./(RHOS*AT)
      AISPS=(PS*AT+C3*VELS)/(9.807*C3)
      WRITE(6,9900)
      WRITE(6,9910) AISPS,TS,PS,RHOS,VELS
      WRITE(6,9840) W
      WRITE(6,9410)
      WRITE(6,9820) (XA(1),I=1,6)
      WRITE(6,9830) (EMUA(I),I=1,6)
      WRITE(6,9100)
      STOP
 9100 FORMAT(1X,130(1H*))
 9200 FORMAT(1X,48HTHE RESULTS OF THE ADIABATIC FLAME ANALYSIS ARE:)
 9300 FORMAT(1X,16HTHE PRESSURE IS ,G13.6,3X,
     *            19HTHE TEMPERATURE IS ,G13.6)
 9400 FORMAT(1X,23HTHE MOLE FRACTIONS ARE ,6(G13.6,2X))
 9410 FORMAT(1X,28X,2HH2,13X,3HH2O,12X,1HH,14X,1HO,14X,2HOH,13X,2HO2)
 9800 FORMAT(1X,35HTHE POST COMBUSTION CONDITIONS ARE:)
 9810 FORMAT(1H0,14HTEMPERATURE = ,G13.6,3X,11HPRESSURE = ,G13.6,3X,
     *            6HRHO = ,G13.6,3X,11HMACH NO. = ,G13.6,3X,
     *            11HVELOCITY = ,G13.6)
 9820 FORMAT(1X,23HTHE MOLE FRACTIONS ARE ,6(G13.6,2X))
 9830 FORMAT(1X,24HTHE NUMBER OF MOLES ARE ,6(G13.6,2X))
 9840 FORMAT(1X,24HTHE MOLECULAR WEIGHT IS ,G13.6)
 9900 FORMAT(1X,26HTHE THROAT CONDITIONS ARE:)
 9910 FORMAT(1H0,10HIMPULSE = ,G13.6,3X,14HTEMPERATURE = ,G13.6,3X,
     *            11HPRESSURE = ,G13.6,3X,6HRHO = ,G13.6,3X,
     *            11HVELOCITY = ,G13.6)
 9920 FORMAT(1H1,51HTHE RESULTS FOR EQUILIBRIUM EXPANSION TO THE THROAT)
 9930 FORMAT(1H1,49HTHE RESULTS FOR IDEAL GAS EXPANSION TO THE THROAT)
      END
      FUNCTION ATDET(GAMMA,EM,ASOAN)
      GM1O2=.5*(GAMMA-1.)
      GF1=.5*(GAMMA+1.)/(GAMMA-1.)
      GF2=ALOG(.5*(GAMMA+1.))
      VAL=ALOG(EM)+GF1*(GF2-ALOG(1.+GM1O2*EM*EM))
      ASOAN=EXP(VAL)
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      ATDET=VAL
      RETURN
      END
      SUBROUTINE EQUIL(ICNST)
      DIMENSION ALAMJ(2)
      COMMON /SPEDAT/EMUA(6),HA(6),GA(6),GPA(6),DHDTA(6),XA(6),
     *                 AJ(2),PHI(6)
      COMMON /CONST/ATCO(2,6),A(2,7,6),WA(6),C1,C2,C3,C4,C5
      COMMON /STATE/T,P,W,H,S,SP,DHDT
      COMMON /MISC/AC,AT,GAMMA
      LOOP1=0
   10 ALAMJ(1)=-.5*(GA(1)+PHI(1))
      ALAMJ(2)=-(GA(2)-GA(1)+PHI(2)-PHI(1))
      DO 20 I=3,6
      IF(I.EQ.ICNST) GOTO 20
      ARG=-(GPA(I)+PHI(I)+ALAMJ(1)*ATCO(1,I)+ALAMJ(2)*ATCO(2,I))/C2
      EMUA(I)=(EXP(ARG))/(P*W)
   20 CONTINUE
      SUM=0.
      DO 30 I=3,6
      SUM=SUM+EMUA(I)*ATCO(2,I)
   30 CONTINUE
      EMUA(2)=(AJ(2)-SUM)/ATCO(2,2)
      SUM=0
      DO 40 I=2,6
      SUM=SUM+EMUA(I)*ATCO(1,I)
   40 CONTINUE
      EMUA(1)=(AJ(1)-SUM)/ATCO(1,1)
      SUM=0.
      DO 50 I=1,6
      IF (EMUA(I).LT..000001) EMUA(I)=.000001
      SUM=SUM+EMUA(I)
   50 CONTINUE
      W=1./SUM
      DO 60 I=1,6
      XA(I)=W*EMUA(I)
   60 CONTINUE
      LOOP1=LOOP1+1
      IF (LOOP1.LT.5) GOTO 40
      RETURN
      END
      SUBROUTINE HSOFT(SPA)
      DIMENSION SPA(6)
      COMMON /SPEDAT/EMUA(6),HA(6),GA(6),GPA(6),DHDTA(6),XA(6),
     *                 AJ(2),PHI(6)
      COMMON /CONST/ATCO(2,6),A(2,7,6),WA(6),C1,C2,C3,C4,C5
      COMMON /STATE/T,P,W,H,S,SP,DHDT
      COMMON /MISC/AC,AT,GAMMA
C     COMPUTE, GIVEN A TEMPERATURE, THE ENTHALPY AND ENTROPY (AT 1 ATM)
C     FOR EACH OF THE SPECIES.
      KR=1
      IF(T.LT.1000.) KR=2
      DO 100 I=1,6
      A1=A(KR,1,I)
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```
      A2=A(KR,2,I)
      A3=A(KR,3,I)
      A4=A(KR,4,I)
      A5=A(KR,5,I)
      A6=A(KR,6,I)
      A7=A(KR,7,I)
      HP=A1+(A2/2.+(A3/3.+(A4/4.+(A5/5.)*T)*T)*T)*T+A6/T
      SP=A1*ALOG(T)+(A2+(A3/2.+(A4/3.+(A5/4.)*T)*T)*T)*T
      SP=SP+A7
      HA(I)=C2*T*HP
      SPA(I)=C2*SP
      DHDTA(I)=C2*(A1+(A2+(A3+(A4+A5*T)*T)*T)*T)
  100 CONTINUE
      RETURN
      END
      SUBROUTINE HASA
      DIMENSION SPA(6),SA(6)
      COMMON /SPEDAT/EMUA(6),HA(6),GA(6),GPA(6),DHDTA(6),XA(6),
     *                AJ(2),PHI(6)
      COMMON /CONST/ATCO(2,6),A(2,7,6),WA(6),C1,C2,C3,C4,C5
      COMMON /STATE/T,P,W,H,S,SP,DHDT
      COMMON /MISC/AC,AT,GAMMA
C     ENTHALPY AND SYSTEM ENTROPY ARE DETERMINED KNOWING T,P,EMUA
      CALL HSOFT(SPA)
      H=0.
      S=0.
      SUM=0.
      DHDT=0.
      DO 100 I=1,6
      SUM=SUM+EMUA(I)
  100 CONTINUE
      W=1./SUM
      DO 200 I=1,6
      H=H+EMUA(I)*HA(I)
      SA(I)=SPA(I)-C2*ALOG(W*EMUA(I)*P)
      GA(I)=HA(I)/T-SA(I)
      GPA(I)=HA(I)/T-SPA(I)
      S=S+EMUA(I)*SA(I)
      DHDT=DHDT+EMUA(I)*DHDTA(I)
  200 CONTINUE
      RETURN
      END
      SUBROUTINE DATAIN
      COMMON /SPEDAT/EMUA(6),HA(6),GA(6),GPA(6),DHDTA(6),XA(6),
     *                AJ(2),PHI(6)
      COMMON /CONST/ATCO(2,6),A(2,7,6),WA(6),C1,C2,C3,C4,C5
      COMMON /STATE/T,P,W,H,S,SP,DHDT
      COMMON /MISC/AC,AT,GAMMA
      READ(5,9100) PF,TF
      READ(5,9200) (XA(I),I=1,6)
      W=0.
      DO 100 I=1,6
      W=W+XA(I)*WA(I)
  100 CONTINUE
```

```
      DO 200 I=1,6
      EMUA(I)=XA(I)/W
  200 CONTINUE
      T=TF
      P=PF
      CALL HASA
      HF=H
      SF=S
      WRITE(6,9300) HF,SF
      WRITE(6,9400) W
      DO 400 J=1,2
      AJ(J)=0.
      DO 300 I=1,6
      AJ(J)=AJ(J)+ATCO(J,I)*EMUA(I)
  300 CONTINUE
  400 CONTINUE
      WRITE(6,9500) (AJ(J),J=1,2)
      READ(5,9600) AC,AT,GAMMA
      WRITE(6,9700) AC,AT,GAMMA
      RETURN
 9100 FORMAT(2E10.2)
 9200 FORMAT(6E10.2)
 9300 FORMAT(1H0,22HTHE TOTAL ENTHALPY IS ,G13.6,3X,
     *          21HTHE FLAME ENTROPY IS ,G13.6)
 9400 FORMAT(1X,24HTHE MOLECULAR WEIGHT IS ,G13.6)
 9500 FORMAT(1X,25HTHE NUMBER OF H ATOMS IS ,G13.6,3X,
     *         25HTHE NUMBER OF O ATOMS IS ,G13.6)
 9600 FORMAT(3E10.2)
 9700 FORMAT(1X,22HTHE COMBUSTOR AREA IS ,G13.6,3X,
     *         19HTHE THROAT AREA IS ,G13.6,3X,
     *         27HTHE ISENTROPIC EXPONENT IS ,G13.6)
      END
      SUBROUTINE DATSET
      COMMON /SPEDAT/EMUA(6),HA(6),GA(6),GPA(6),DHDTA(6),XA(6),
     *             AJ(2),PHI(6)
      COMMON /CONST/ATCO(2,6),A(2,7,6),WA(6),C1,C2,C3,C4,C5
      COMMON /STATE/T,P,W,H,S,SP,DHDT
      COMMON /MISC/AC,AT,GAMMA
C
C     SET THE ATOMIC COEFFICIENTS FOR THE MOLECULAR SPECIES
C     THE ARRAY ATCO(J,I) CONTAINS THE NUMBER OF ATOMS OF ATOMIC SPECIES J
C     CONTAINED IN MOLECULAR SPECIES I. THERE ARE SIX MOLECULAR SPECIES
C     TREATED. THEY ARE (IN ORDER) H2,H2O,H,O,OH,O2. ATOMIC SPECIES ARE H,O.
      ATCO(1,3)=1.
      ATCO(2,3)=0.
      ATCO(1,1)=2.
      ATCO(2,1)=0.
      ATCO(1,2)=2.
      ATCO(2,2)=1.
      ATCO(1,4)=0.
      ATCO(2,4)=1.
      ATCO(1,5)=1.
      ATCO(2,5)=1.
      ATCO(1,6)=0.
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```
      ATCO(2,6)=2.
C     IN THE FOLLOWING BLOCK THE THERMODYNAMIC COEFFICIENTS FOR EACH OF THE
C     MOLECULAR SPECIES ARE SET. THEY ARE STORED IN A(K,J,I) WHERE J=1,7 FOR
C     EACH OF THE MOLECULAR SPECIES I=1,6. THE K INDEX IDENTIFIES THE
C     TEMPERATURE RANGE (1=HIGH,2=LOW).
C     H DATA FOLLOWS
      A(2,1,3)=.25E+01
      A(2,2,3)=0.
      A(2,3,3)=0.
      A(2,4,3)=0.
      A(2,5,3)=0.
      A(2,6,3)=.25471627E+05
      A(2,7,3)=-.46011762
      A(1,1,3)=.25E+01
      A(1,2,3)=0.
      A(1,3,3)=0.
      A(1,4,3)=0.
      A(1,5,3)=0.
      A(1,6,3)=.25471627E+05
      A(1,7,3)=-.46011763
C     H2 DATA FOLLOWS
      A(2,1,1)=.30574451E+01
      A(2,2,1)=.267652E-02
      A(2,3,1)=-.58099162E-05
      A(2,4,1)=.55210391E-08
      A(2,5,1)=-.18122739E-11
      A(2,6,1)=-.98890474E+03
      A(2,7,1)=-.22997056E+01
      A(1,1,1)=.31001901E+01
      A(1,2,1)=.51119464E-03
      A(1,3,1)=.5264421E-07
      A(1,4,1)=-.34909973E-10
      A(1,5,1)=.369453345E-14
      A(1,6,1)=-.87738042E+03
      A(1,7,1)=-.19629421E+01
C     H2O DATA FOLLOWS
      A(2,1,2)=.40701275E+01
      A(2,2,2)=-.11084499E-02
      A(2,3,2)=.41521180E-05
      A(2,4,2)=-.29637404E-08
      A(2,5,2)=.80702103E-12
      A(2,6,2)=-.30279722E+05
      A(2,7,2)=-.32270046
      A(1,1,2)=.27167633E+01
      A(1,2,2)=.29451374E-02
      A(1,3,2)=-.80224374E-06
      A(1,4,2)=.10226682E-09
      A(1,5,2)=-.484721453E-14
      A(1,6,2)=-.29905826E+05
      A(1,7,2)=.66305671E+01
C     O DATA FOLLOWS
      A(2,1,4)=.29464287E+01
      A(2,2,4)=-.16381665E-02
      A(2,3,4)=.24210316E-05
```

```
      RETURN
      END
      SUBROUTINE ITSUB(X,FOFX,NITSUB,CONV,SAVEIT)
      DIMENSION SAVEIT(8)
C                 ITERATION CONTROL SUBROUTINE ...FINDS X SUCH THAT F(X)=0
C                 MAIN PROGRAM MUST DIMENSION SAVEIT(8)
C                 CALLING PROGRAM COMPUTES (GIVEN AN X) FOFX AND ALSO
C                 SUPPLIES CONVERGENCE CRITERION (CONV) AND # OF ITERATIONS
C                 (NITSUB)...ITSUB THEN CONTROLS SUBSEQUENT VALUES OF X
C                 INITALIZE ITSUB BY SETTING SAVEIT(1)=1
C                 SET AMOUNT TO PERTURB X BY IN SAVEIT(2)
      IF((ABS(FOFX)-CONV).LE.0.) GOTO 730
      ITIME=IFIX(SAVEIT(1)+.1)
      GOTO (330,380,470,570),ITIME
  330 CONTINUE
      ITIME=2
      SAVEIT(3)=1.
      FOFXCK=FOFX
      SAVEIT(8)=FOFXCK
      IF(FOFX.LT.0.) GOTO 470
  380 CONTINUE
      IF(FOFX.LT.0.) GOTO 570
      IF(FOFXCK.GE.FOFX) GOTO 430
      SAVEIT(2)=-SAVEIT(2)
      X=X-2.*SAVEIT(2)
      GOTO 670
  430 CONTINUE
      SAVEIT(4)=X
      SAVEIT(5)=FOFX
      X=X-SAVEIT(2)
      GOTO 670
  470 CONTINUE
      ITIME=3
      IF(FOFX.GT.0.) GOTO 570
      IF(FOFXCK.LE.FOFX) GOTO 530
      SAVEIT(2)=-SAVEIT(2)
      X=X+2.*SAVEIT(2)
      GOTO 670
  530 CONTINUE
      SAVEIT(6)=X
      SAVEIT(7)=FOFX
      X=X+SAVEIT(2)
      GOTO 670
  570 CONTINUE
      ITIME=4
      IF(FOFX.LT.0.) GOTO 630
      SAVEIT(4)=X
      SAVEIT(5)=FOFX
      GOTO 650
  630 CONTINUE
      SAVEIT(6)=X
      SAVEIT(7)=FOFX
  650 CONTINUE
      X=SAVEIT(4)-SAVEIT(5)*(SAVEIT(6)-SAVEIT(4))/(SAVEIT(7)-SAVEIT(5))
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      IF((X-SAVEIT(4))*(X-SAVEIT(6)).GT.0.) GOTO 710
  670 CONTINUE
      NTEMP=IFIX(SAVEIT(3)+.1)
      IF(NTEMP.GE.NITSUB) GOTO 710
      NTEMP=NTEMP+1
      SAVEIT(3)=FLOAT(NTEMP)
      GOTO 780
  710 CONTINUE
      ITIME=6
      GOTO 780
  730 CONTINUE
      ITIME=5
      SAVEIT(4)=X
      SAVEIT(5)=FOFX
      SAVEIT(6)=X
      SAVEIT(7)=FOFX
  780 CONTINUE
      SAVEIT(1)=FLOAT(ITIME)
      RETURN
      END
```