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EVALUATION OF
ON-BOARD HYDROGEN STORAGE METHODS
FOR HIGH-SPEED AIRCRAFT
(NAG-1-767)

STATUS REPORT
January 31, 1991

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(NASA-CR-187755) EVALUATION OF ON-BOARD
HYDROGEN STORAGE METHODS FOR HIGH-SPEED
AIRCRAFT Status Report (Hampton Univ.)
95 p CSCL 01C N91-22121
63/05 Unclas 0012316

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ABSTRACT

Hydrogen is the fuel of choice for hypersonic vehicles. Its main disadvantage is its low liquid and solid density. This increases the vehicle volume and hence the drag losses during atmospheric flight. In addition, the dry mass of the vehicle is larger due to larger vehicle structure and fuel tankage. Therefore it is very desirable to find a fuel system with smaller fuel storage requirements without deteriorating the vehicle performance substantially.

To evaluate various candidate fuel systems, they were first screened thermodynamically with respect to their energy content and cooling capacities. To evaluate the vehicle performance with different fuel systems, a simple computer model is developed to compute the vehicle parameters such as the vehicle volume, dry mass, effective specific impulse, and payload capacity.

The results indicate that if the payload capacity (or the gross lift-off mass) is the most important criterion, only slush hydrogen and liquid hydrogen - liquid methane gel shows better performance than the liquid hydrogen vehicle. But if all the advantages of a smaller vehicle is considered and a more accurate mass analysis can be performed, other systems using endothermic fuels such as cyclohexane, and some boranes may prove to be worthy of further consideration.

INTRODUCTION

Hydrogen is a foremost candidate as a fuel for use in hypersonic flight. The National Aerospace program has been initiated by NASA and the Department of Defense for developing hypersonic / transatmospheric vehicles for takeoff from conventional airport runways to orbit, or for rapid, long distance, intercontinental aerospace transportation. For this purpose, air-breathing, hydrogen fueled supersonic combustion ramjet (scramjet) engines are being developed for speeds of Mach 5 to 25.

The main difficulty encountered in the use of hydrogen as a fuel for hypersonic vehicles is the large volume required for its on-board storage. If hydrogen is stored as liquid, it requires about four times the volume to produce the same amount of energy as conventional fuels. This is especially important for supersonic and hypersonic vehicles which need to have slender designs to reduce drag losses.

Initially the objective of this study was to identify and evaluate the storage media capable of increasing the hydrogen storage density (mass of hydrogen stored per unit storage volume) to a level higher than that of liquid hydrogen (70 kg/m^3). It was then realized that since the fuel system and the vehicle formed a complex system, any improvement in the hydrogen density would involve several trade-offs. For this reason, the establishment of a set of criteria for the evaluation of various fuel systems and putting together a model which will make a quantitative evaluation possible became the primary objective of this work.

EVALUATION CRITERIA

During hypersonic flight, beside providing propulsion, the fuel has to contribute to structural and engine cooling. In addition, combustibles other than hydrogen in the fuel system may serve as rocket fuel during the final stage of flight to orbit and for maneuvering in space, or they may be burnt to provide power for the vehicle subsystems. Therefore, the hydrogen storage density, the

heats of combustion of hydrogen and other combustibles in the fuel system, and the cooling capacity of the fuel and the storage system are important parameters in the evaluation of candidate fuel systems.

It should also be realized that for any improvement in hydrogen storage density a certain penalty has to be paid in terms of increased mass, decreased specific impulse, or increased cost and complexity of tankage, fuel feed systems and technology development. Increase in fuel mass may be at least partially compensated by decreases in some mass components such as the tankage mass and thermal protection mass. Decrease in the specific impulse may be offset by a decrease in drag losses so that the effective specific impulse may not be reduced as much as the specific impulse. These effects depend on, among others, the flight trajectory, whether the plane is designed as a launch vehicle or as a hypersonic transport plane, the structural design, the type of engines to be used, and the switchover Mach numbers for the engines. Only the first two effects are considered in the present work. To account for them, differences in the effective specific impulses and the payload capacities are taken to be the additional evaluation criteria.

In order to quantify the basis for the evaluation of the candidate fuel systems they are first thermodynamically screened with respect to their hydrogen density, energy content, and cooling capacities. The most promising systems are then evaluated using the developed model in terms of the payload capacities and effective specific impulses of the corresponding vehicles. The results of the thermodynamic evaluation are given in Appendix A, the flow chart for the computer model is presented in Appendix B, the computer program is included in Appendix C, information on the computer program is in Appendix D, and the results of some computations are included in Appendix E.

MODELING CONSIDERATIONS

At the start of this study the only tools available to us for the comparison of the performances of vehicles with different structures and engines were the ongoing work by Dorrington¹ on alpha-beta relationships and the ASP computer program developed at NASA Langley Research Center² for the assessment of the effects of component size changes on the aircraft performance. The former was still under development and the latter could only be applied to vehicles with turbojet - ramjet engines using liquid hydrogen or methane and was limited to Mach numbers less than 4.5. Recently, we became aware of a similar study done for the Air Force Wright Research and Development Center by Aerojet TechSystems and Boeing Aerospace, which used inhouse codes for engine analysis and trajectory optimization and compared the performances of vehicles using a variety of fuels based on ammonia and boron hydrides to the performance of a vehicle using slush hydrogen. The dissemination of this information was restricted and therefore, it did not have much influence on the present study.

Since the design of NASP is not finalized yet, there is no need to accurately predict the performance of a certain hypothetical vehicle. The purpose of this study will be better served by a simple model which can compare the payload capacity and effective specific impulse of various vehicles to those of a vehicle using liquid hydrogen. To achieve this we used the conceptual design approach of chemical process design. Accordingly we started with the simplest possible model and added details and complexities step by step until the model produced sufficient information of acceptable accuracy.

The starting model only considered the hypersonic air-breathing phase of the flight. The reasoning was that during the subsonic - supersonic phase all the vehicles could use identical engines and fuels if they had the same gross lift off mass. The mass change was calculated by a macroscopic energy balance similar to the approach used by Jones and Donaldson³, which used a specified thrust

to drag ratio to account for the drag losses. The initial thrust to drag ratio was assumed to be the same for all vehicles and it is used to determine the engine size which is assumed to be fixed. The thrust and drag (and, hence, their ratio) were allowed to change during the hypersonic flight. The specific impulse was calculated at the beginning and at the end of the hypersonic phase. The details of the engine was not considered. The combustion chamber pressure was determined by specifying a compression ratio. Products of constant pressure combustion at equilibrium was determined by the chemical equilibrium code developed by NASA Lewis Research Center. Exit velocities were computed by assuming frozen expansion in an ideal nozzle to ambient pressure. All vehicles were assumed to have the same gross lift off mass and any weight penalty manifested itself as reduced payload capacity. This enabled several mass components such as the thrust structure mass and the engine mass which are functions of the initial vehicle mass to be the same for all vehicles and simplified the analysis considerably.

This initial model failed to discriminate effectively between vehicles with different fuel systems due to its various shortcomings. The problems and the way they are dealt with in the final program are summarized below:

1. If chemical binding is used to increase hydrogen storage density, the extra mass introduced should replace an equal amount of mass that already exists on board the vehicle to prevent a reduction in the payload capacity. One method which seemed feasible was the possibility of using the extra mass as the rocket fuel for the final stage of flight after the extraction of hydrogen to be used as the air breathing phase fuel. For this purpose a section was added to the program to evaluate the performance of the rocket phase and compute the fuel requirements. This phase of the flight was assumed to be free of drag losses. Instead of assuming a specific impulse and calculating the mass ratio using this specific impulse, a macroscopic energy balance was used to obtain the mass

ratio and the specific impulse was then calculated using this information. This was done to account for different specific impulses of different fuels.

2. Since the vehicle sizes will be different due to different fuel volumes, the drag encountered by each vehicle will be different. In order to account for this the hypersonic flight phase was investigated in more detail. The initial simple model was used to find the mass ratio for the subsonic-supersonic phase. Since the same average thrust to drag ratio is used for all vehicles, the vehicles with smaller drag will have a larger thrust during this first phase. This will affect the required engine and thrust structure masses. At this level of sophistication of the model this effect is ignored. It was also assumed that the vehicles to be compared will have the same thrust to drag ratio at the commencement of the hypersonic flight phase. From this information the thrust and the capture area for each vehicle is obtained and assumed to be fixed for the entire flight. The effective specific impulse is computed at each 100 m altitude step and after every 10 steps the differential equation giving the mass ratio for the interval was integrated numerically.

Since there is no data against which the results of the proposed model can be checked, the ability of the model to represent the performance of a hypersonic vehicle can be verified only by checking if the magnitude and the variation of quantities such as thrust, drag, and specific impulse are technically reasonable. The introduction of details mentioned above also provided information which were used for this purpose.

3. The original model used a specified compression ratio to calculate the combustion chamber pressure and could not account for the effect of Mach number on forebody compression. In the final model a more realistic approach is used. The forebody and engine geometry used is taken from Ikawa⁴ and his method is used to obtain

the conditions at the combustion chamber exit. For the aftbody expansion we kept the simplifying assumption of isentropic, frozen expansion.

4. In the initial model the drag coefficient for the vehicle was taken to be dependent only on the angle of attack. Since the omission of the Mach number dependence produced unsatisfactory drag and thrust profiles, the equation used to obtain the drag coefficients is modified to include Mach number dependence. This is done by fitting an equation to the curve given by Dorrington².

5. The initial model was modified to allow the specification of varying dynamic pressures and angle of attack values during the hypersonic flight phase. At the present, three different values can be specified at three selected flight Mach numbers. The program can easily be changed to increase this number.

The flow chart for the final model is given in Appendix B and the program listing in Appendix C.

RESULTS

The results for some potential fuel systems are summarized in Table 1. The entries in this table are the differences from the corresponding values for a vehicle using liquid hydrogen as fuel for the entire flight. These results were obtained for a fixed set of conditions given below:

Dynamic pressure = 47882 Pa (1000 lb_f/ft²)

Gross lift-off mass = 300,000 kg

Orbital altitude = 200,000 m

Orbital velocity = 8030 m/s

Angle of attack = 2 degrees

Switchover Mach number for hypersonic propulsion = 3

Switchover Mach number for rocket propulsion = 12

Table 1.

Comparison of hypersonic vehicles using various fuel systems with the vehicle using liquid hydrogen. Negative sign indicates a value lower than that of the LH2 vehicle.

Fuel System			Difference in vehicle volume (%)	Difference in dry mass (%)	Difference in payload capacity (%)	Approximate difference in GLOW (%)	Difference in effective specific impulse (Mach 3-12 range) (%)
First phase fuel	Second phase fuel	Third phase fuel					
SH2	SH2	SH2	- 11	- 3.2	+ 7.2	- 1.8	+ 1.2 to + 2.9
CH4	CH4	CH4	- 50	- 18	- 80	+ 20	- 53 to - 66
CH4-H2	CH4-H2	CH4-H2	- 12	- 3.8	+ 0.6	- 0.14	- 3.6 to - 3.2
CH4	H2	CH4	- 48	- 15	- 55	+ 13	+ 5.4 to + 13
CH4	NH3	CH4	- 48	- 19	- 89	+ 22	- 76 to - 53
C3H8	NH3B5H9	C3H8	- 56	- 20	- 89	+ 22	- 69 to - 63
CH4	H2	CO	CO cannot be used alone as the rocket phase fuel.				
LH2	H2(C6H12)	C6H6	- 8.6	- 11	- 83	+ 20	+ 0.9 to + 2.3
LH2	H2(C7H14)	C7H8	- 8.0	- 11	- 83	+ 20	+ 0.8 to + 2.1
LH2	H2(B2H6)	B	- 16	- 9.1	- 50	+ 12	+ 1.7 to + 4.2
LH2	H2(ALH3)	AL	- 34	- 16	- 96	+ 24	+ 3.7 to + 9.3
LH2	H2(LIH)	LI	- 17	- 11	- 75	+ 18	+ 1.8 to + 4.5
LH2	H2(NH3B5H9)	BN	- 19	- 19	- 129	+ 32	+ 2.0 to + 5.1
LH2	H2(NH3B10H13)	BN	- 2.7	- 16	- 131	+ 32	+ 0.3 to + 0.8
LH2	H2(N2H5B5H9)	BN	- 19	- 18	- 129	+ 32	+ 2.0 to + 5.1

Only two systems show a net improvement over the liquid hydrogen vehicle. Slush hydrogen gives the best performance providing a 11% decrease in vehicle volume and a 7.2% increase in payload capacity (or about 2% decrease in gross lift off mass). Liquid methane - liquid hydrogen gel results in a similar decrease in vehicle volume, but provides only a 0.6% increase in payload capacity (or about 0.14% decrease in the gross lift off mass). For the other systems, there is a trade-off between an appreciable decrease in vehicle volume and an increase in the gross lift-off mass. Among these, the so called endothermic fuels appear to have a lot of potential because they provide a means for returning some of the energy that was lost through dissipation as heat, back to the system. For this reason, an important aspect in the use of endothermic fuels is matching the cooling duty to the endothermicity of the fuel. One drawback for the use of these fuels is the additional mass of the reactor and the catalyst that needs to be carried on board.

Among the endothermic fuels investigated, diborane appears to provide the best payload capacity but it is still only about one half the capacity of a liquid hydrogen vehicle. The vehicle using diborane will have 12% more gross lift-off mass but it will be 16% smaller and its dry mass will be about 9% lighter. Lithium hydride produces similar results. The use of cyclohexane as an endothermic fuel results in 8.6% decrease in vehicle volume and 11% decrease in dry mass in return for 83% reduction of payload capacity or 20% increase in gross lift-off mass.

Another set of fuel systems studied uses a different fuel for each flight phase. Use of methane, for example, instead of hydrogen in the first air breathing phase and in the final rocket propulsion phase produces a drastic decrease in the vehicle volume (48%) in return for a 55% decrease in the payload capacity (or a 13% increase in the gross lift-off mass).

Methane, methanol, and jet fuel reforming, plausible source of hydrogen for hypersonic propulsion provided that the carbon monoxide produced can be used as fuel for rocket propulsion. The heat of combustion of carbon monoxide is too small to be used as a rocket fuel for the final phase by itself, but it can be mixed with some hydrogen before it is sent to the rocket engines. In addition to the extra mass of the reactor and the catalyst some water must also be carried on board as a reactant. Of course, a gaseous rocket fuel such as CO will involve an additional storage problem because the gaseous rocket fuel produced during air breathing propulsion cannot be used immediately. Because of these drawbacks it is quite unlikely that reforming may become a possible source of hydrogen for hypersonic flight.

As more information on the temperature and heat flux distribution on the vehicle surface become available it will be possible to find better endothermic fuels to maximize energy recovery. In addition, since the final decision will involve a trade-off between smaller vehicle volume and dry mass versus a smaller gross lift-off mass, the relative improvements in these should be assigned weights to point out the best system to be used. If the gross lift-off mass is the most important factor, then the best fuel to be used is the slush hydrogen. But if the decrease in the vehicle volume and dry mass can be converted into significant savings in some mass components such as engine mass, propellant tankage mass, and thrust structure mass endothermic fuels such as boron hydride may prove to be superior provided that the boron produced can be burned in the rocket engines. Evaluation of this possibility cannot be done before accurate correlations for various mass components in terms of vehicle parameters become available.

RECOMMENDATIONS

The following modifications to the model are recommended to enhance the ability of the model to predict the relative merits of different fuel systems. Of course the trade-off will be between the more realistic predictions on one hand and the increased time and effort required to develop and run a more sophisticated model.

1. Rather than using an average thrust to drag ratio for the subsonic-supersonic flight phase, a more detailed analysis of this phase may be incorporated to the model so that it can handle different shapes, engines, and trajectories for vehicles with different fuel systems. At this point the best way to accomplish this is to create an interface between the current model and the ASP code that already exists at the NASA Langley Research Center. This modification may make the model too long to run even on a microcomputer with 486, 25 MHz processor.

2. Trajectory optimization may also be included for the hypersonic phase, but the increase in run time may be prohibitive for a PC based program.

3. The hypersonic phase model may be modified to include off design performance of fixed geometry engines and the use of variable geometry engines. At this point it is not clear if the improvement in the ability of the model to discriminate between vehicles with different fuel systems will warrant the extra effort and time required for this modification.

4. In the present computer code the final rocket propulsion phase is analyzed by a simple energy balance incorporating a specified propulsion efficiency. Since the results indicate that the calculated payload capacity is sensitive to the propellant requirement of this phase of flight, it is recommended that a more accurate analysis of the rocket phase be made by using the rocket option of the NASA/Lewis chemical equilibrium code to obtain the specific impulse.

5. In the present model the final phase of flight using rockets is assumed to occur without any drag due to high altitude and short time of flight. But, in order to optimize the switchover Mach number, incorporation of the effect of drag in rocket phase calculations is essential. This can be done by correcting the calculated specific impulse for drag losses to obtain the effective specific impulse, and using this effective specific impulse to obtain the mass ratio for the rocket phase.

6. Cooling during hypersonic flight is an essential function of any fuel system. Different fuel systems will have different weight requirements for the accomplishment of this cooling duty, and, therefore, this mass difference may be critical in the selection of an appropriate fuel system. Incorporation of realistic estimates of the cooling system masses will be very beneficial but, at this point this appears to be difficult to accomplish.

7. More realistic correlation of different system masses with vehicle parameters will increase the accuracy of the model.

8. A parametric study of the model should be performed to determine the sensitivity of the results to the values of the vehicle and flight parameters. Subsequently more realistic values or correlations should be introduced for the important parameters.

9. Most importantly, in the selection of the fuel systems for consideration, it was assumed that the part of the fuel remaining after the removal of hydrogen can be burnt in the rocket engines for the final phase of flight. This needs to be checked for technical possibility.

10. The computer program has gone through numerous modifications and has not been optimized yet for efficiency. This should be done before any of the above recommendations are implemented.

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APPENDIX A

Evaluation of Hydrogen Storage Media

Fuel System	Hydrogen Density Kg H ₂ /m ³	Total Combustion Energy		Combustion Energy (due to hydrogen)		Cooling Capacity	
		Mj/kg	MJ/m ³	MJ/kg	MJ/m ³	MJ/kg	MJ/m ³
I.							
Liquid Hydrogen	70.0	120.0	8400	120.0	8400	0.400	28.0
Hydrogen Slush (50% Solid)	80.9	120.00	9400	-	-	0.430	34.8
Liquid Methane	-	50.0	20900	-	-	0.505	211.0

II.

Endothermic Fuels

A. Hydrocarbons

1. Cyclohexane	56.0	46.4	36100	8.7	6710	2.80	2200
2. Methylcyclohexane	47.4	45.9	35300	7.5	5750	2.40	1860
3. Decalin	65.3	43.2	38700	8.8	8060	2.70	2400
4. Methane reforming with							
i) H ₂ O ⁽¹⁾	107.4	29.6	17900	21.3	13000	7.60	4580
ii) CO ₂	53.3	17.5	13900	8.1	6370	4.50	3580
5. Ammonia	121.2	21.3	14500	21.3	14700	4.10	2790
6. Methanol dissociation	99.8	23.9	18900	15.4	12200	3.90	3120
7. Ammonia-Borane	-	39.6	-	23.3	-	0.80	-

Fuel System	Hydrogen Density Kg H ₂ /m ³	Total Combustion Energy		Combustion Energy (due to hydrogen)		Cooling Capacity	
		Mj/kg	MJ/m ³	MJ/kg	MJ/m ³	MJ/kg	MJ/m ³
B. Metal Hydrides							
1. Magnesium							
a. MgH ₂	109	32.0	45600	9.2	12800	2.7	3790
2. Lithium							
a. LiH	98.5	52.7	41200	15.2	12100	11.3	8840
3. Titanium							
a. TiH _{1.97}	150.5	22.7	86400	4.7	16100	2.5	9370
4. Aluminum							
a. AlH ₃	151.2	40.1	60100	12.2	18300	0.4	628
5. Zirconium							
a. ZrH ₂	122.2	14.2	80300	2.6	14700	1.9	10750
6. Lanthanum							
a. La Ni ₅ H ₆	89	7.0	45900	1.6	10100	0.06	366

III.

Slurries with Liquid H₂

1. MgH₂

a. H ₂ : 25% (by mass)	75	54.3	13200	37.1	9050	2.1	510
b. H ₂ : 50%	71.8	76.5	10200	65.1	8680	1.5	204
c. H ₂ : 75%	70.6	98.8	9060	93.1	8550	1.0	88

2. LiH

a. H ₂ : 25% (by mass)	76	69.5	15300	41.7	9200	8.8	1940
b. H ₂ : 50%	72.3	86.8	11100	68.1	8750	6.1	780

Fuel System	Hydrogen Density Kg H ₂ /m ³	Total Combustion Energy		Combustion Energy (due to hydrogen)		Cooling Capacity	
		Mj/kg	MJ/m ³	MJ/kg	MJ/m ³	MJ/kg	MJ/m ³
c. H ₂ : 75%	70.80	103.9	9400	94.6	8570	3.1	280
3. TiH ₂							
a. H ₂ : 25% (by mass)	74.2	47.3	12500	33.8	8980	1.9	504
b. H ₂ : 50%	71.5	71.9	9900	62.9	8650	1.4	193
c. H ₂ : 75%	70.5	96.4	8900	91.9	8530	0.9	83
4. Al H ₃							
a. H ₂ : 25% (by mass)	80	60.0	14750	39.4	9680	0.4	98.3
b. H ₂ : 50%	73.6	80.0	10700	66.6	8910	0.4	53.5
c. H ₂ : 75%	71.2	100.0	9200	93.8	8620	0.4	36.7
5. Zr H ₂							
a. H ₂ : 25% (by mass)	71.9	40.9	11000	32.2	8690	1.5	405
b. H ₂ : 50%	70.6	67.6	9300	61.8	8550	1.2	166
c. H ₂ : 75%	70.2	94.3	8800	91.4	8490	0.8	74
6. NH ₃ • BH ₃							
a. H ₂ : 25% (by mass)	+	60.0	+	48.0	-	0.7	+
b. H ₂ : 50%	-	80.3	-	72.4	-	0.6	-
c. H ₂ : 75%	-	100.7	-	96.7	-	0.5	-

IV.

Cryogenic Adsorption

1. Activated Carbon	18-25	41.0	15000	8.2	3000	0.03	10
2. Silica Gel	22.3	3.8	2700	3.8	2700	0.013	8.9

Fuel System	Hydrogen Density Kg H ₂ /m ³	Total Combustion Energy		Combustion Energy (due to hydrogen)		Cooling Capacity	
		Mj/kg	MJ/m ³	MJ/kg	MJ/m ³	MJ/kg	MJ/m ³
3. Nickel Oxide-Silicate	19.6-22.8	4.1	2700	4.1	2700	0.014	9.1

V.

Mixture of Liquid H₂ with ignition promoters

1. Aluminum Borohydride (Al(BH ₄) ₃) 20% by (mass)	70.66	107.6	9120	100.9	8550	0.32	27.1
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VI.

Mixtures of Liquid H₂ with Endothermic Fuels and Jet Fuels

1. Cyclohexane

a. H ₂ :95% (by mass)	69.93	116.3	8530	114.4	8392	0.52	38.1
b. H ₂ :90%	69.86	112.6	8674	108.9	8383	0.64	49.3
c. H ₂ :85%	69.78	109.0	8833	103.3	8374	0.76	61.6
d. H ₂ :75%	69.59	101.6	9207	92.2	8351	1.00	90.6

2. Methylcyclohexane

a. H ₂ :95% (by mass)	69.89	116.3	8528	114.4	8387	0.5	36.7
b. H ₂ :90%	69.77	112.6	8669	108.7	8373	0.6	46.2
c. H ₂ :85%	69.64	108.9	8825	103.1	8357	0.7	56.7
d. H ₂ :75%	69.33	101.5	9192	91.9	8320	0.9	81.5

3. Decalin

a. H ₂ :95% (by mass)	69.98	116.2	8524	114.4	8398	0.52	37.8
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Fuel System	Hydrogen Density Kg H ₂ /m ³	Total Combustion Energy		Combustion Energy (due to hydrogen)		Cooling Capacity	
		Mj/kg	MJ/m ³	MJ/kg	MJ/m ³	MJ/kg	MJ/m ³
b. H ₂ :90%	69.96	112.3	8661	108.9	8395	0.63	48.6
c. H ₂ :85%	69.94	108.5	8812	103.3	8392	0.75	60.5
d. H ₂ :75%	69.88	100.8	9169	92.2	8386	0.98	88.7
4. JP-4							
a. H ₂ :95% (by mass)	69.66	116.2	8519	114	8359	0.38	27.9
b. H ₂ :90%	69.29	112.4	8650	108	8315	0.36	27.7
c. H ₂ :85%	68.88	108.5	8794	102	8266	0.34	27.6
d. H ₂ :75%	67.92	100.9	9135	90	8150	0.30	27.2
5. JP-5							
a. H ₂ :95% (by mass)	69.68	116.2	8520	114	8362	0.38	27.9
b. H ₂ :90%	69.34	112.3	8652	108	8321	0.36	27.7
c. H ₂ :85%	68.96	108.5	8798	102	8275	0.34	27.6
d. H ₂ :75%	68.05	100.8	9142	90	8167	0.30	27.2
6. JP-10							
a. H ₂ :95% (by mass)	69.73	116.1	8522	114	8367	0.38	27.9
b. H ₂ :90%	69.42	112.2	8656	108	8331	0.36	27.8
c. H ₂ :85%	69.09	108.3	8804	102	8291	0.34	27.6
d. H ₂ :75%	68.30	100.5	9155	90	8196	0.30	27.3

VII.

Gelation of Liquid Hydrogen

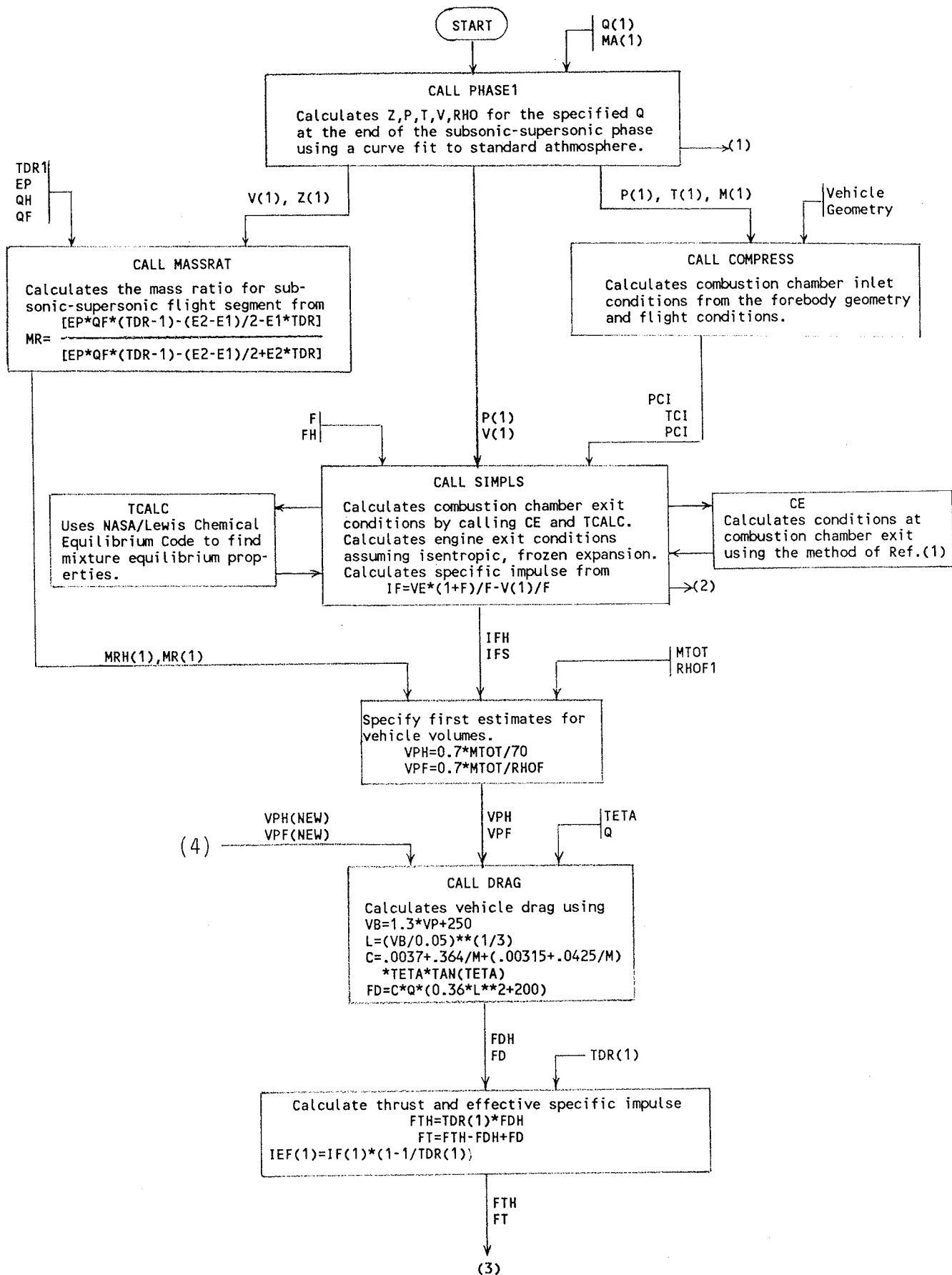
1. Carbon Black

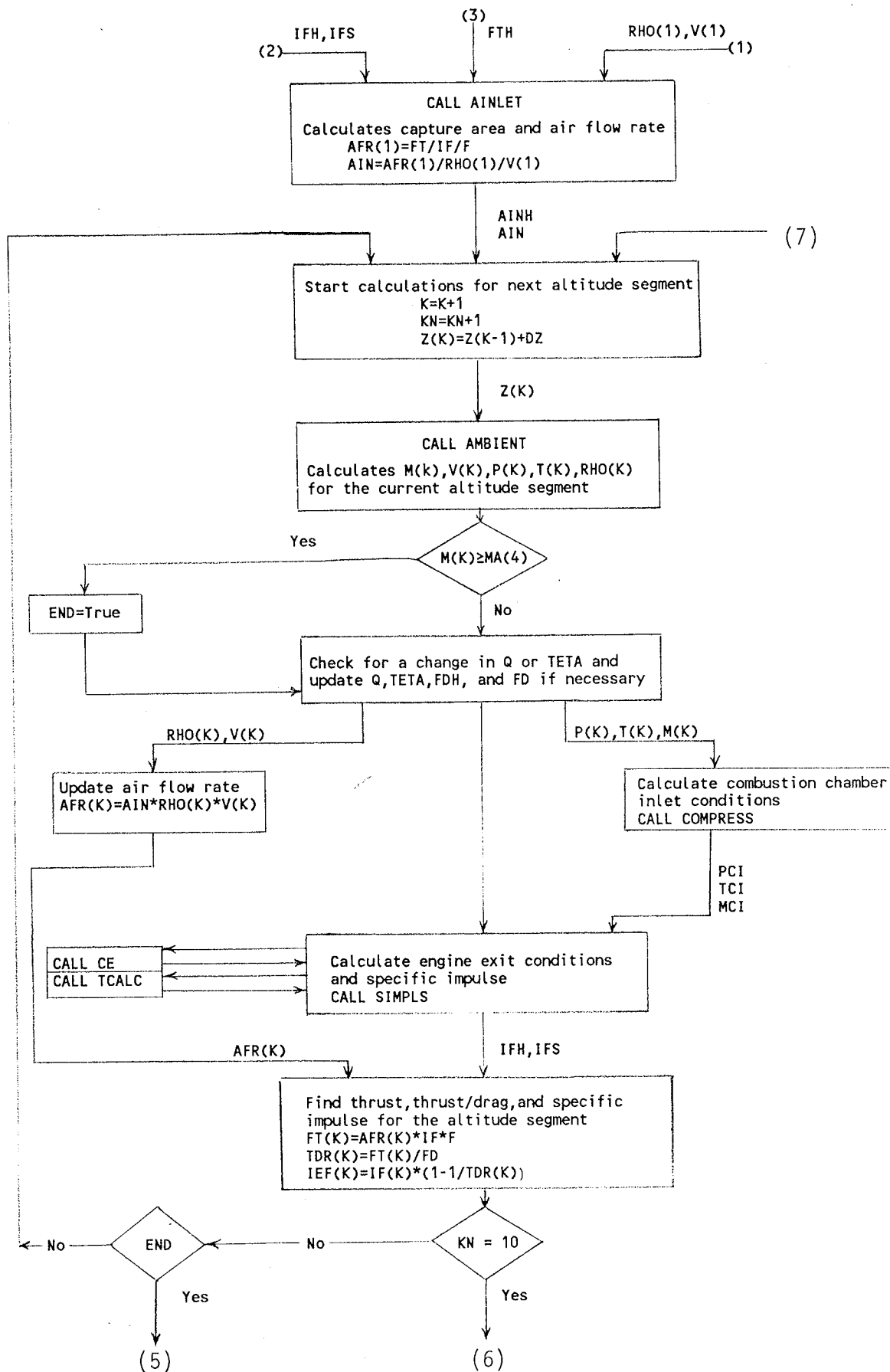
H ₂ :72% (by mass)	69.02	95.58	9295	86.4	8400	0.288	28
-------------------------------	-------	-------	------	------	------	-------	----

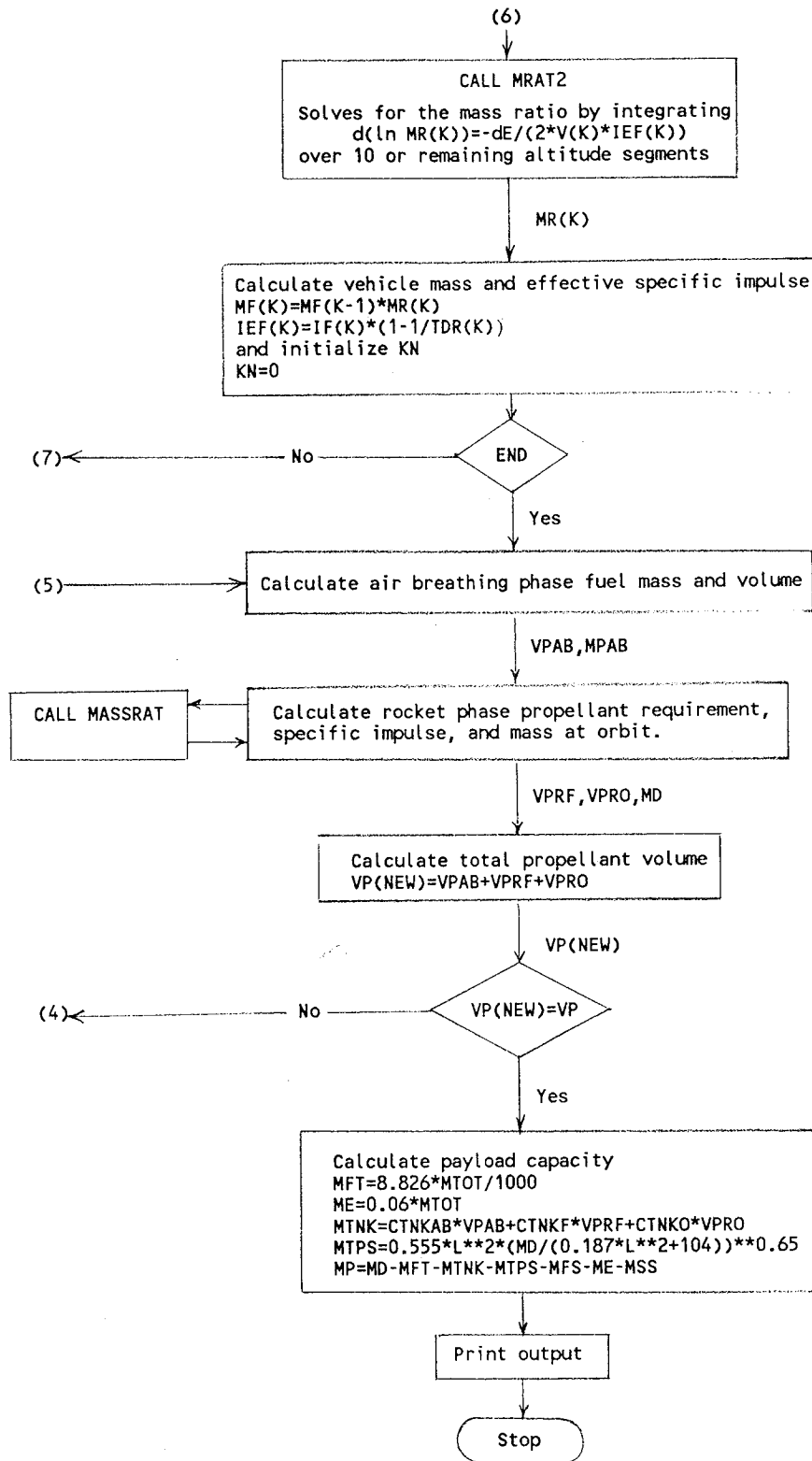
Fuel System	Hydrogen Density Kg H ₂ /m ³	Total Combustion Energy		Combustion Energy (due to hydrogen)		Cooling Capacity	
		Mj/kg	MJ/m ³	MJ/kg	MJ/m ³	MJ/kg	MJ/m ³
2. Pyrogenic Silica							
H ₂ :62.3% (by mass)	68.67	74.76	8240	74.76	8240	0.26	27.5
3. LiALH ₄							
a. H ₂ :14% (by mass)	79.09	53.5	18290	27.75	9490	2.71	926.2
b. H ₂ :90	70.24	112.3	8659	109.3	8428	0.668	51.55
4. LiBH ₄							
a. H ₂ :33% (by mass)	77.31	67.8	11545	54.8	9277	5.99	1020
b. H ₂ :80%	71.23	104.4	8886	100.4	8548	2.07	176
c. H ₂ :90%	70.80	112.2	8649	110.2	8496	1.23	95
5. Aluminum Flake							
H ₂ :27%	64.75	55.1	13214	32.4	7769.5	0.108	25.9
6. CH ₄							
a. H ₂ :83%	67.58	108.1	8801.5	99.6	8109	0.42	34.0
b. H ₂ :91.5%	78.41	114.05	9773	109.8	9409	0.44	37.4
7. Boron							
H ₂ :90% (by mass)	69.77	109.27	8469	108	8371	0.36	27.90
8. LiH							
H ₂ :90%	70.32	112.3	8653	109.5	8438	1.49	114.9
9. Li ₂ C ₂ H ₂ :90%	69.67	111.5	8631	108	8360	0.36	27.87
10. Diborane							
H ₂ :90%	68.78	115.1	8795	108	8254	0.36	27.51
11. Pentaborane							
H ₂ :90%	69.13	114.7	8807.5	108	8296	0.36	27.65

Fuel System	Hydrogen Density Kg H ₂ /m ³	Total Combustion Energy		Combustion Energy (due to hydrogen)		Cooling Capacity	
		Mj/kg	MJ/m ³	MJ/kg	MJ/m ³	MJ/kg	MJ/m ³
12. Decaborane							
H ₂ :90%	69.43	114.6	8838	108	8331	0.36	27.77
13. Ammonia							
H ₂ :90%	69.12	110.2	8459	110	8458	0.77	59.09
14. Ethane							
a. H ₂ :95% (by mass)	69.53	116.6	8534	114	8344	0.38	27.81
b. H ₂ :90%	69.02	113.2	8681	108	8282	0.36	27.61
c. H ₂ :85%	68.45	109.8	8842	102	8214	0.34	27.38
15. Suspension with Cyclopropane							
H ₂ :90%	69.25	109.4	8418	108	8310	0.36	27.7

APPENDIX B







APPENDIX C

PROGRAM EVAL

11:15 am FRI 2. 15. 1991
16:12:35 Sat 16-Feb-1991

IMPLICIT REAL (A-I,L-Z)
LOGICAL HTEST,END2,CONV,WRT,NOPRT,tptest
INTEGER FTEST
CHARACTER RUN*4, FUEL*10

DIMENSION Z(400),Q(4),MA(4),M(400),V(400),P(400),T(400),
+ RHO(400),TDR(400),ISH(400),IFH(400),IS(400),IFS(400),
+ TETA(3),FTH(400),TDRH(400),AFRH(400),AFR(400),MRH(400),
+ MR(400),MFH(400),MF(400),IEFFH(400),FT(400),FUEL(4),
+ IEFF(400),ZC(4),KK(10),IEFH(400),IEF(400),DH(400),D(400)

COMMON/FLG/JPH1,HTEST,WRT,JQ
COMMON/PROP/QH,QF,QF1,EP,EPR,QRR,Qfr
COMMON PI
COMMON/COMB/PCI,MCI,TCI,rci,vci,tpptest
COMMON/DNS/rhoce,pce,GAMAce,SVELce,OFRRAT,hce,tce,cpce
common/mxt/a,b,xkc,fm,gm,alf,bet,trat
common /mas/ieffh,ieff,v,z

DATA VORB/8030./,CTNKH/9.2/,CTNKO/8.3/,END2/.FALSE./,ORB/200./

PI=3.141593
CONV=.FALSE.
JQ=0
OPEN(UNIT=1,FILE='NMLST.DAT')
OPEN(UNIT=2,FILE='EVAL.GIN')
OPEN(UNIT=3,FILE='EVAL.FIN')
OPEN(UNIT=4,FILE='THERMO.DAT')
OPEN(UNIT=5,FILE='EVAL.HIN')
OPEN(UNIT=6,FILE='EVAL.OUT')

If FTEST= 1, same fuel is used in the first and second phases of A-B flight and they both contribute to rocket propulsion.

If FTEST = 2, fuel for the first phase supplies the fuel for the second phase and contributes to rocket propulsion.

If FTEST = 3, rocket propulsion is independent of A-B fuel and A-B fuel is used directly.

If FTEST = 4, hydrogen is used in the first A-B phase and partially in the second A-B phase. A second fuel is used to produce the rest of the second A-B phase hydrogen and all of the rocket phase fuel.

N is the ratio of the mass of rocket fuel obtained during A-B propulsion per unit mass of A-B fuel produced.

EM is the ratio of fuel system mass (excluding tankage) to the mass of A-B fuel produced (for ftest=1 and 2).

QF = Heat of combustion of second A-B phase fuel
QF1 = Heat of combustion of first A-B phase fuel

QRR = Heat of combustion of rocket fuel produced during A-B phase
QFR = Heat of combustion of additional rocket fuel

RHOH = Density of baseline fuel
RHOF = Density of second A-B phase fuel (density of hydrogen source
for FTEST = 4)
RHOF1 = Density of first A-B phase fuel
RHOFR = Density of additional rocket fuel

F = Fuel to air mass ratio for A-B phase fuel
FRR = Fuel to oxygen mass ratio for rocket fuel produced during
A-B phase
FFR = Fuel to oxygen mass ratio for the additional rocket fuel

CTNK1 = Tankage mass per unit propellant volume for the first
A-B phase fuel.
CTNK2 = Tankage mass per unit propellant volume for the second
A-B phase fuel (for FTEST = 4, this is for the fuel
producing the rocket fuel and supplementary hydrogen).
CTNKF = Tankage mass per unit propellant volume for the
additional rocket fuel.

```
READ(2,10) RUN,FUEL(1),FUEL(2),FUEL(3),fuel(4)
Read (2,15) FTEST,NOPRT,wrt
Read (2,17) mtot,mssh,mssf,rhoh,epr
READ(2,20) MA(1),MA(2),MA(3),MA(4)
READ(2,20) (Q(J),J=1,4)
READ(2,22) (TETA(J),J=1,3)
READ(2,30) TDR1,TDR(1),TDRH(1),DZ
READ(2,40) QH,QF1,QFR,QF,QRR,EP
READ(2,42) FRR,FFR,N,EM
READ(2,50) CTNKF,CTNK1,CTNK2,RHOF,RHOF1,RHOFR
10 FORMAT(A4,4A10)
15 format(I2,2L7)
17 format(5e12.6)
20 FORMAT(4F8.3)
22 FORMAT(3F8.3)
30 FORMAT(3F10.6,E12.6)
40 FORMAT(6E12.6)
42 FORMAT(4E12.6)
50 FORMAT(6F10.6)
WRITE(6,51)RUN,(FUEL(J),J=1,4),FTEST,NOPRT,(MA(J),J=1,4),(Q(J),
+ J=1,4),(TETA(J),J=1,3),TDR1,TDR(1),TDRH(1),DZ,QH,QF1,QFR,QF,
+ QRR,EP,FRR,FFR,N,EM,ep,epr,CTNKF,CTNK1,CTNK2,RHOF,RHOF1,RHOFR
51 FORMAT(5X,'*** ',70X,'ATES AKYURTLU ***' // '-----
+-----' //36X,'** INPUT **'//2X,'
+RUN = ',A4/3X,' FUEL = ',4(A10,5X)/3X,' FTEST = ',I2,5X,' NOPRT = ',
+L7/3X,' MA = ',4G12.6/3X,' Q (PA)=',4G12.6/3X,' TETA (DEG)=',3G12.6
+/3X,' TDR1 = ',G12.6,5X,' TDR(1) = ',G12.6,5X,' TDRH(1) = ',G12.6,5X
+,' DZ (M)=',G12.6/3X,' QH (J/KG)=',G12.6,2X,' QF1 (J/KG)=',G12.6,2X
+,' QFR (J/KG)=',G12.6,2X,' QF (J/KG)=',G12.6,2X,' QRR (J/KG)=',G12.6
+/3X,' EP = ',G12.6,5X,' FRR = ',G12.6,5X,' FFR = ',G12.6,5X,' N = ',G12.6
+/3X,' FUEL SYSTEM MASS/FUEL MASS(EM)=',G12.6,5x,' EP = ',G12.6,5X,
+' EPR = ',G12.6/3X,' CTNKF = ',G12.6
+,5X,' CTNK1 = ',G12.6,5X,' CTNK2 = ',G12.6/3X,' RHOF (kg/m3)=',
+ G12.6,5x,' RHOF1 (kg/m3)=',G12.6,5X,' RHOFR (kg/m3)=',G12.6,5X
+ // '-----
+-----')
```

LEWIND 2
JPH1 = 0

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OF POOR QUALITY

CALL PHASE1 (Q(1),MA(1),Z(1),M(1),V(1),P(1),T(1),RHO(1))

C
IF (JPH1.NE.0) THEN
WRITE (6,100) JPH1
100 FORMAT (1H ,/1X,'*** NO CONVERGENCE IN',I3,' TRIALS. PHASE1 COULD
+NOT BE EXECUTED.***')
GOTO 1000
ENDIF

C
C
C IF(JMR=0) QQ=QF1, IF(JMR=1) QQ=QH, IF(JMR=2) QQ=QF, IF(JMR=3)
C ROCKET PROPULSION
C

JMR=1
CALL MASSRAT (JMR,TDR1,0.,0.,V(1),Z(1),MRH1)
JMR=0
CALL MASSRAT (JMR,TDR1,0.,0.,V(1),Z(1),MR1)

C
K=1

C
CALL COMPRES (P(K),M(K),T(K))

C
HTEST = .TRUE.

C
CALL SIMPLS (V(K),P(K),FH,ISH(K),IFH(K))

C
HTEST = .FALSE.

C
CALL SIMPLS (V(K),P(K),F,IS(K),IFS(K))

C
TETAR = TETA(1) * PI/180.0
MFH(1) = MRH1*MTOT
MF(1)=MR1*MTOT
VPH = 0.6*mtot/RHOH
VPF = 0.6*mtot/RHOF
JH = 0

C
170 CONTINUE

C
CALL DRAG (TETAR,Q(1),VPH,FDH,m(k))

C
FTH(1) = TDRH(1) *FDH

C
CALL AINLET (Rho(1),v(1),FTH(1),ISH(1),FH,AINH,DINH)

C
CALL DRAG (TETAR,Q(1),VPF,FD,m(k))

C
FT(1) = FTH(1)-FDH+FD

C
IEFFH(K)= IFH(K)*(1.0-1.0/TDRH(K))
IEFF(K) = IFS(K)*(1.0-1.0/TDR(K))
IEFH(K)= ISH(K)*(1.0-1.0/TDRH(K))
IEF(K) = IS(K)*(1.0-1.0/TDR(K))

C
CALL AINLET (Rho(1),v(1),FT(1),IS(1),F,AIN,DIN)

```
      Q=Q(1)
      k1=k
      kn=1
190 K=K+1
      kn=kn+1
      Z(K) = Z(K-1) +DZ
C
      CALL AMBIENT (Z(K),QQ,M(K),V(K),P(K),T(K),RHO(K))
C
      IF (M(K).GE.MA(4)) END2=.TRUE.
      IF(NOPRT) GOTO 195
      IF(CONV.AND.END2) WRT=.TRUE.
195 CONTINUE
      do 200 j=1,3
      IF (M(K).GE.MA(J)) THEN
      TETAR = TETA(J) *PI/180.
      QQ = Q(J+1)
C
      call drag(tetar,qq,vph,fdh,m(k))
C
      call drag(tetar,qq,vpf,fd,m(k))
C
      endif
200 CONTINUE
C
      CALL COMPRES (P(K),M(K),T(K))
C
      AFRH(K)= AINH*Rho(k) *V(k)
      AFR(K) = AIN *Rho(k) *V(k)
      HTEST = .TRUE.
C
      CALL SIMPLS (V(K),P(K),FH,ISH(K),IFH(K))
C
      HTEST = .FALSE.
C
      CALL SIMPLS (V(K),P(K),F,IS(K),IFS(K))
C
      FTH(K)=AFRH(K) *ISH(K) *(1.+FH)
      FT(K) = AFR(K)*IS(K)*(1.+F)
      TDRH(K)=FTH(K)/FDH
      TDR(K)=FT(K)/FD
      TDRMH = (TDRH(K) + TDRH(K-1))/2.0
      TDRM = (TDR(K) + TDR(K-1))/2.0
C
      mfh(k)=mfh(k-1)
      mf(k)=mf(k-1)
      IEFFH(K)= IFH(K)*(1.0-1.0/TDRH(K))
      IEFF(K) = IFS(K)*(1.0-1.0/TDR(K))
      IEFH(K)= ISH(K)*(1.0-1.0/TDRH(K))
      IEF(K) = IS(K)*(1.0-1.0/TDR(K))
C
      if(kn.eq.10) then
      JMR=1
      CALL MRAT2(JMR,k1,k,MRH(K))
C
      JMR=2
      CALL MRAT2(JMR,k1,k,MR(K))
C
      MFH(K) = MFH(K-1) *MRH(K)
      MF(K) = MF(K-1) *MR(K)
```



```
  . = k+1
kn=0
IEFFH(K) = IFH(K)*(1.0-1.0/TDRH(K))
IEFF(K) = IFS(K)*(1.0-1.0/TDR(K))
IEFH(K) = ISH(K)*(1.0-1.0/TDRH(K))
IEF(K) = IS(K)*(1.0-1.0/TDR(K))
endif
IF(END2) GOTO 300
GOTO 190
300 KEND=K
  if(kn.eq.0) goto 295
  jmr=1
  CALL MRAT2(JMR,k1,k,MRH(K))
  jmr=2
  CALL MRAT2(JMR,k1,k,MR(K))
  MFH(K) = MFH(K-1) *MRH(K)
  MF(K) = MF(K-1) *MR(K)
295 continue
  MABH = MFH(KEND)
  MABF = MF(KEND)
  VPHAB = (MTOT-MABH)/RHOH
  DV = VORB - V(KEND)
  ZORB = ORB*1000.
303 JMR=3
  HTEST = .TRUE.
  CALL MASSRAT (JMR,TDRM,V(KEND),Z(KEND),VORB,ZORB,MRRH)
  ISRH = DV/ALOG(1./MRRH)/9.813
  MDH = MRRH*MABH
  VPHH = VPH
  FRH = FH/0.22840
  VPHRF = (MABH - MDH)/(FRH + 1.0)*(FRH/RHOH)
  VPHRO = (MABH - MDH)/(FRH+1.0)/1140.
  DVPHR = VPHRF + VPHRO
  VPH = VPHAB + DVPHR
  VPFF = VPF
c
c      EXFL = Amount of rocket fuel produced during A-B phase in
c      excess of the actual rocket phase requirement.
c
EXFL = 0.0
c
IF (FTEST .EQ. 1) THEN
c
  vpfab = (mtot-mabf)*(1.+n)/rhofl
  MFRAB = N*(MTOT-MABF)
  mfs = em*(mtot-mabf)
c
ELSEIF (FTEST .EQ. 2) THEN
  vpfab = (mtot-mf(1))/rhofl + (mf(1)-mabf)*(1.+n)/rhofl
  MFRAB = N*(MF(1)-MABF)
  mfs = em*(mf(1)-mabf)
endif
  if (ftest.eq.3) goto 310
c
  If QR = QRR , jq = 0
c
  If QR = QFR , jq = 1
c
  If QR = QF1 , jq = 2
c
jq=0
jmr=3
```

```

EST=.FALSE.
call massrat(jmr,1.,v(kend),z(kend),vorb,zorb,mrr)
mdf=mrr*mabf
mfrckt =(mabf-mdf)*frr/(1.+frr)
if (ftest.eq.4) then
vpf1=(mtot-mf(1))/rhof1
vpf2h=(mf(1)-mabf-mfrckt/n)/RHOH
vpf2f=mfrckt*(n+1.)/n/rhof
vpf2=vpf2h+vpf2f
vpfab=vpf1+vpf2
mfs=em*mfrckt/n
mfrab=mfrckt
endif
if (mfrab.ge.mfrckt) then
exfl = mfrab-mfrckt
mfrf = 0.0
mfro = mfrckt/frr
else
mrr1 = (mabf-mfrab*(frr+1.)/frr)/mabf
e1 = v(kend)**2/2.+z(kend)*9.7
e2 = (ep*qrr*(1.-mrr1)-e1)/mrr1
e1 = e2
e2 = vorb**2/2.+zorb*9.2
mrr2 = (ep*qfr-e1)/(ep*qfr+e2)
mrr = mrr1*mrr2
mdf = mabf*mrr
mfrf = -(mdf-mabf*mrr1)*ffr/(1.+ffr)
mfro = mfrf/ffr+mfrab/frr
endif
ISR=DV/ALOG(1./MRR)/9.813
goto 320

```

310 continue

c

```

vpf2 = -(mabf-mf(1))/rhof1
VPF1 = (mtot-mf(1))/rhof
VPFAB= VPF1+VPF2
jq=1
HTEST=.FALSE.
CALL MASSRAT (JMR,TDRM,V(KEND),Z(KEND),VORB,ZORB,MRR)
mdf = mabf*mrr
mfrf = (mabf-mdf)*ffr/(1.+ffr)
mfro = mfrf/ffr
ISR=DV/ALOG(1./MRR)/9.813
mfs = 0.0

```

320 continue

```

VPFRF = MFRF/RHOFR
VPFRO = MFRO/1140.
VPFR=VPFRF + VPFRO
VPF = VPFAB + VPFR
ERPH = ABS(VPH-VPHH)/VPH
ERPF = ABS(VPF-VPFF)/VPF
IF(CONV) GOTO 350
IF((ERPH .LT. 0.05).AND.(ERPF .LT. 0.05)) then
CONV=.TRUE.
if (noprt) goto 350
endif
JH = JH+1
IF(JH.GT.100) GOTO 340
K=1
END2=.FALSE.

```

ofo 170
 WRITE (6,345) JH
 345 FORMAT(1H /'***ERROR. VP DOES NOT CONVERGE IN', I3,' ITERATIONS' /)
 350 CONTINUE
 WRITE(6,355) JH
 355 FORMAT(1H /5X,'*** VP CONVERGED IN ',I3,' ITERATIONS ***' /)

MFTH = 8.826 *MTOT/1000.
 MTNKH = CTNKH * (VPH + VPHRF) + CTNKO * VPHRO

CALL LENGTH (VPH,LH,VBH)

MTPSH = 0.555 * LH **2 * (MDH/(0.187*LH**2+104.0))**0.65
 MTH = MFTH + MTNKH + MTPSH
 ME = 0.06 * MTOT
 MPH = MDH-MTH-ME-MSSH
 MFTF = 8.826 * MTOT/1000.0
 IF(FTEST.LT.3) THEN
 MTNKF = CTNK1*VPFAB+ CTNKF * VPRFR +CTNKO * VPFRO
 ELSEIF (FTEST.EQ.3) THEN
 MTNKF=CTNK1*VPF1+CTNK2*VPF2+CTNKF*VPRFR+CTNKO*VPFRO
 ELSEIF (ftest.eq.4) THEN
 mtnkf=ctnk1*vpf1+ctnk2*vpf2f+ctnkh*vpf2h+ctnko*vpfro
 ENDIF

CALL LENGTH (VPF,L,VPF)

MTPSF = 0.555*L**2*(MDF/(0.187*L**2+104.0))**0.65
 MTF = MFTF + MTNKF +MTPSF+mfs
 mdf = mdf-exfl
 MPF = MDFF-MTF-ME-MSSF
 DO 360, JL=2,4

CALL PHASE1(Q(JL),MA(JL),ZC(JL),XM,XV,XP,XT,XR)

IF (JPH1.NE.0) THEN
 WRITE (6,100) JPH1
 ENDIF

360 CONTINUE
 ZC(1)=Z(1)
 MPROPH=MTOT-MDH
 MPROPF=MTOT-MDF
 DO 399, J=1,KEND
 DH(J)=FTH(J)/TDRH(J)
 D(J)=FT(J)/TDR(J)

399 CONTINUE

AFRH(1)= AINH*RHO(1) *V(1)
 AFR(1) = AIN *RHO(1) *V(1)

WRITE(6,400) RUN,FUEL(4),(JF,FUEL(JF),JF=1,3),MTOT,ORB,VORB
 400 FORMAT(1H /1X,'-----'
 +,'-----',
 + '-----' //5X,' RUN NUMBER =',A4//5X,' BASELINE FUEL ='
 +',A10//3(5X,' PHASE ',I1,' FUEL = ',A10//5X,' LIFT-OFF MASS = ',
 +G12.6,' KG' /5X,' ORBITAL ALTITUDE = ',G12.6,' KM' /
 +5X,' ORBITAL VELOCITY = ',G12.6,' M/S' /1X,
 + '-----'
 + '-----')
 WRITE(6,405)

```

FORMAT(1H /42X,'** VEHICLE PARAMETERS **'//40X,'BASE VEHICLE',
+5X,'VEHICLE RUNNING'/39X,'RUNNING ON H2',4X,'ON TEST FUEL(S)'/
+39X,'-----',3X,'-----')
406 Format(5X,'A-B phase fuel volume (m3)',9x,2(3x,g12.6)/5x,'Rocket p
+phase propellant volume (m3)',2(3x,g12.6)/5x,'Total vehicle volume
+(m3)',10x,2(3x,g12.6)/5x,'Characteristic dimension (m)',7x,2(3x,g1
+2.6)/5x,'Mass of vehicle at orbit (kg)',6x,2(3x,g12.6)/5x,'Mass of
+ vehicle at switchover (kg)',1x,2(3x,g12.6)/5x,'A-B phase fuel mas
+s (kg)',11x,2(3x,g12.6)/5x,'Rocket propellant mass (kg)',8x,2(3x,g
+12.6)/5x,'Rocket fuel produced (kg)',14x,'.000000',7x,g12.6/5x,'Ad
+ditional rocket fuel (kg)',12x,'.000000',7x,g12.6/5x,'Excess rocke
+t fuel (kg)',16x,'.000000',7x,g12.6/5x,'Total propellant mass cons
+umed (kg)',2(3x,g12.6)/5x,'Thrust structure mass (kg)',9x,2(3x,g12
+.6)/5x,'Propellant tankage mass (kg)',7x,2(3x,g12.6)/5x,'Fuel Prod
+uction system mass (kg)',7x,'.000000',7X,G12.6/5x,'Thermal protect
+ion mass (kg)',7x,2(3x,g12.6)/5x,'Engine mass (kg)',19x,2(3x,g12.6
+)/5x,'Subsystem mass (kg)',16x,2(3x,g12.6)
+/5x,'Payload mass (kg)',18x,2(3x,g12.6)/5x,'Rocket specific impuls
+e (s)',8x,2(3x,g12.6)/5x,'Capture area (m2)',18x,2(3x,g12.6)/)

```

```

mpabh = mtot-mabh
mpabf = mtot-mabf
mprh = mabh-mdh
mprf = mabf-mdf
if(ftest.eq.3) mfrf=0.0

```

```

WRITE(6,406) vphab,vpfab,dvphr,vpfr,VBH,vbf,LH,L,MDH,mdf,mabh,
& mabf,mpabh,mpabf,mprh,mprf,mfrab,mfrf,exfl,MPROPH,mpropf,mfth,
& mftf,mtnkh,mtnkf,mfs,mtpsh,mtpsf,me,me,MSSH,MSSF,MPH,mpf,isrh,
& isr,ainh,ain

```

```
WRITE(6,410)
```

```

410 FORMAT(1H /36X,'** FLIGHT PROFILE **'//15X,'PHASE1 AB',10X,
+ 'CHANGE TO',12X,
+ 'PHASE2 AB',13X,'CHANGE TO'/34X,'HYPERSONIC',36X,'ROCKET'/
+14X,'-----',8X,'-----',3X,'-----'
+-',3X,'-----')

```

```

WRITE(6,420) (ZC(KC),KC=1,4),(MA(KC),KC=1,4),(Q(KC),KC=1,4),
+ (TETA(KC),KC=1,3)

```

```

420 FORMAT(1H /1X,'Z (M)',28X,G12.6,3X,G12.6,3X,G12.6,3X,G12.6/1X,
+'MA',31X,G12.6,3(3X,G12.6)/1X,'Q (PA)',8X,G12.6,8X,
+G12.6,3X,G12.6,3X,G12.6/1X,'TETA (DEG)',23X,G12.6,2(3X,G12.6)/)
WRITE(6,425)

```

```

425 FORMAT(1H , '-----'
+-----'//36X,'** HYPERSONIC PHASE PROFILE **'// ' ',11X,' ',12X,' '
+ SPECIFIC ' ', ' SPECIFIC ' ',2X,
+' EFF. FUEL ' ',1X,' EFF. FUEL ' '/
+' ' ALTITUDE ' ',12X,' 'IMPULSE, H2' ', ' IMPULSE,FUEL' ',
+' SPEC. IMPULS' ', ' SPEC. IMPULS' '
+/' ' ',4X,' (M)' ',4X,' 'MACH NUMBER' ',4X,' (S)' ',5X,
+' ' ',4X,' (S)' ',5X,' ' ',1X
+', ' H2, (S) ' ', ' FUEL, (S) ' '
+/' '-----', ' '-----', ' '-----', ' '-----',
+' '-----', ' '-----')

```

```

426 FORMAT(1H , '-----'
+', '-----',
+', '-----'//2X,' ALTITUDE' ',
+16X,' THRUST/DRAG' ',2X,' THRUST/DRAG' ',4X,' DRAG' ',9X,' DRAG' ',8X,
+' THRUST' ',7X,' THRUST' ',6X,' AIR FLOW' ',

```

```

      X, 'AIR FLOW' /5X, ' (M)' ,5X, 'MACH NUMBER' ,1X, 'RATIO, H2' ,3X,
+ 'RATIO, FUEL' ,
+4X, ' H2, (N)' ,5X, ' FUEL, (N)' ,4X, ' H2, (N)' ,5X, ' FUEL, (N)' ,3X,
+ ' H2, (KG/S)' ,2X, ' FUEL, (KG/S)' /' -----' ,1X, '-----' ,
+ 1X, '-----' ,1X, '-----' ,1X, '-----' ,1X,
+ '-----' ,1X, '-----' ,1X, '-----' ,1X,
+ '-----' ,1X, '-----' /)

```

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C

```

DO 431, J=1, KEND
IFH(J)=IFH(J)/9.813
IFS(J)=IFS(J)/9.813
IEFFH(J)=IEFFH(J)/9.813
IEFF(J)=IEFF(J)/9.813
431 CONTINUE
KK(1)=1
IF(KEND.LT.10) GOTO 440
DO 430, J=1, 8
KK(J+1)=KK(J)+KEND/10
430 CONTINUE
DO 435, KW=1, 9
JK=KK(KW)
WRITE(6,460) Z(JK), M(JK), IFH(JK), IFS(JK),
+ IEFFH(JK), IEFF(JK)
435 CONTINUE
WRITE(6,460) Z(KEND), M(KEND), IFH(KEND), IFS(KEND),
+ IEFFH(KEND), IEFF(KEND)
WRITE(6,426)
DO 437, J=1, 8
KK(J+1)=KK(J)+KEND/10
437 CONTINUE
DO 438, KW=1, 9
JK=KK(KW)
WRITE(6,461) Z(JK), M(JK), TDRH(JK), TDR(JK), DH(JK),
+ D(JK), FTH(JK), FT(JK), AFRH(JK), AFR(JK)
438 CONTINUE
WRITE(6,461) Z(KEND), M(KEND), TDRH(KEND), TDR(KEND), DH(KEND),
+ D(KEND), FTH(KEND), FT(KEND), AFRH(KEND), AFR(KEND)
GOTO 1000
440 DO 450, J=1, KEND
KK(J+1)=KK(J)+1
450 CONTINUE
DO 455, KW=1, KEND
JK=KK(KW)
WRITE(6,460) Z(JK), M(JK), IFH(JK), IFS(JK),
+ IEFFH(JK), IEFF(JK)
455 CONTINUE
460 FORMAT(1H G12.6, 3(1X, G12.6), 2X, G12.6, 1X, G12.6)
461 FORMAT(1H G12.6, 7(1X, G12.6), 2X, G12.6, 1X, G12.6)
WRITE(6,460) Z(KEND), M(KEND), IFH(KEND), IFS(KEND),
+ IEFFH(KEND), IEFF(KEND)
WRITE(6,426)
DO 447, J=1, 8
KK(J+1)=KK(J)+KEND/10
447 CONTINUE
DO 448, KW=1, 9
JK=KK(KW)
WRITE(6,461) Z(JK), M(JK), TDRH(JK), TDR(JK), DH(JK),
+ D(JK), FTH(JK), FT(JK), AFRH(JK), AFR(JK)
448 CONTINUE
WRITE(6,461) Z(KEND), M(KEND), TDRH(KEND), TDR(KEND), DH(KEND),

```

```
(KEND), FTH(KEND), FT(KEND), AFRH(KEND), AFR(KEND)  
STOP  
END
```

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```
C  
C  
SUBROUTINE PHASE1 (Q,MA,Z,M,V,P,T,RHO)  
C  
IMPLICIT REAL (A-H,M-Z)  
C  
LOGICAL HTEST,WRT  
COMMON /FLG/JPH1 ,HTEST,WRT,JQ  
C  
ZT=0  
Z = 10000.  
10 CALL AMBIENT(Z,Q,M,V,P,T,RHO)  
JPH1=JPH1+ 1  
RELER=ABS(M-MA)/MA  
IF(RELER.LE.0.001) THEN  
GOTO 20  
ELSEIF(JPH1.GE.100) THEN  
GOTO 30  
ELSEIF(M.LT.MA) THEN  
ZTT=Z  
DZ=5000*(MA/M-1.0)  
Z = Z+DZ  
ZT = ZTT  
GOTO 10  
ELSEIF(M.GT.MA) THEN  
ZTTT=Z  
DZ=5000*(M/MA-1.0)  
Z = Z-DZ  
ZT = ZTTT  
GOTO 10  
ENDIF  
20 CONTINUE  
JPH1=0  
30 RETURN  
END
```

```
C  
C  
SUBROUTINE AMBIENT (Z,Q,M,V,P,T,RHO)  
C  
IMPLICIT REAL (A-H,M-Z)  
C  
A1 = -6535.  
B1 = 1020.  
A2 = -6449.  
B2 = 4238  
IF(Z.GT.35000.)THEN  
A1 = -7787.  
B1 = -5581.  
ENDIF  
IF(Z.GT.45000.)THEN  
A2= -7934.  
B2= -4096.  
ENDIF  
IF(Z.GT.65000.)THEN  
A1= -5729.  
B1= 14340.  
ENDIF
```

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```
(Z.GT.75000.)THEN  
A2 = -5718.  
B2=18048.  
ENDIF  
IF(Z.GT.100000.)THEN  
A1 = -11750  
B1 = -75718  
A2 = -8936.  
B2 = -28632.  
ENDIF  
P = EXP((Z-B1)/A1)*101325.  
RHO = EXP((Z-B2)/A2)  
T = P*0.003483/RHO  
A = SQRT(401.9*T)  
V = SQRT(2.0*Q/RHO)  
M = V/A  
RETURN  
END
```

C
SUBROUTINE SIMPLS (V,P,F,IS,IF)

C
IMPLICIT REAL (A-I,L-Z)
LOGICAL HTEST,WRT,tptest

C
COMMON/FLG/JPH1,HTEST,WRT,JQ
COMMON/COMB/PCI,MCI,TGI,rci,vci,tptest
COMMON/DNS/rhoce,pce,GAMAce,SVELce,OFRAT,hce,tce,cpce
common/mxt/a,b,xkc,fm,gm,alf,bet,trat

C
tpptest=.true.
xkc=1.2
pold=pci
told=tci
mold=mci
call tcalc
gci=gamace
rci=rhoce*1000.
vci=mci*svelce
F=1./OFRAT
cp1=cpce*4186.8
tpptest=.false.
call tcalc
cp2=cpce*4186.8
qtot=cp2*tce-cp1*tci
tti=tci*(1.+0.5*(gci-1.)*mci**2)
tte=tti-tci+tce
trat=tte/tti
g=(gci+gamace)/2.
a=g*(xkc-1.)-xkc
b=2.*xkc-1.
bet=1./b
alf=1.-bet
call ce(mci,tci,pci,g,m2,t2,p2)
tci=t2
pci=p2
mci=m2
tpptest=.true.
call tcalc
gc=gamace
ac=svelce

```

      m2
      vc=mc*ac
      PC=P2
      RHOC=rhoce*1000.
      G1 = GC-1.
      A = (P/PC)**(G1/GC)
      B = 1. +0.5*G1*MC**2
      ME = SQRT(2.*(B-A)/G1/A)
      RHOE = RHOC*(P/PC)**(1./GC)
      AE = SQRT(GC*P/RHOE)
      VE = ME*AE
      IS = (VE-V/(1.+F))
      IF = (IS*(1. + F)/F)

```

```

      pci=pold
      tci=told
      mci=mold
      RETURN
      END

```

```

      subroutine ce(mci,tci,pci,g,m2,t2,p2)
      implicit real (a-h,m-z)
      common/mxt/a,b,xkc,fm,gm,alf,bet, trat
      pold=pci
      call cmexit(mci,g,m2)
      pci=pold
      t2=tci*fm**((b-1.)/b)*gm**((1./b)
      p2=pci*fm**((a+xkc)/a)
      return
      end

```

```

      subroutine cmexit(m1,g,m2)
      implicit real (a-h,m-z)
      common/mxt/a,b,xkc, fm,gm,alf,bet, trat
      m2=m1
      mn22=0.
      m22=m2**2
10  fm=(a*m1**2+b)/(a*m22+b)
      if(fm.lt.0.) then
      m22=(mm22+m22)/2.
      goto 10
      endif
      gm=m1**2/m22
      hm=(1.+0.5*(g-1.)*m22)/(1.+0.5*(g-1.)*m1**2)
      fg=fm**(alf)*gm**bet*hm
      f=trat-fg
      fp=fg*(a*alf/(a*m22+b)+bet/m22-((g-1.)/2.)
      & /(1.+0.5*(g-1.)*m22))
      mn22=m22-f/fp
      reler=abs((mn22-m22)/m22)
      if(reler.lt.0.005) goto 100
      mm22=m22
      m22=mn22
      goto 10
100 m2=sqrt(m22)
      return
      end

```


SUBROUTINE MASSRAT (JMR,TDR,V1,Z1,V2,Z2,MR)

IMPLICIT REAL (A-I,L-Z)

LOGICAL HTEST,WRT

COMMON/PROP/ QH,QF,QF1,EP,EPR,QRR,Qfr

COMMON/FLG/JPH1,HTEST,WRT,JQ

QR=QRR

IF(JQ.EQ.1) QR=QFR

IF(JQ.EQ.2) QR=QF1

IF(HTEST) QR=QH

IF(JMR.EQ.3) THEN

QQ=QR

EP=EPR

E1=V1**2/2.0+Z1*9.7

E2=V2**2/2.0+Z2*9.2

MR=(EP*QQ-E1)/(EP*QQ+E2)

GOTO 10

ENDIF

QQ=QH

IF(JMR.EQ.0) QQ=QF1

IF(JMR.EQ.2) QQ=QF

E1= V1**2/2.0 +Z1*9.8

E2= V2**2/2.0 +Z2*9.8

A = EP*QQ*(TDR-1)-0.5*(E2-E1)

MR= (A-E1*TDR)/(A+ E2 * TDR)

10 CONTINUE

RETURN

END

subroutine mrat2(jmr,k1,k,mr)

implicit real (a-i,l-z)

dimension ieffh(400),ieff(400),v(400),z(400),e(400),f(400),

& esi(400)

common/mas/ieffh,ieff,v,z

int=0.

do 20 j=k1,k

e(j)=v(j)**2+2.*9.7*z(j)

if(jmr.eq.1)then

esi(j)=ieffh(j)

elseif(jmr.eq.2) then

esi(j)=ieff(j)

elseif((jmr.gt.2).or.(jmr.lt.1)) then

write(*,10) jmr

10 format(5x,'ERROR : MASSRAT2 WAS USED WITH JMR =',i2)

stop

endif

f(j)=1./(2.*v(j)*esi(j))

if(j.eq.k1)go to 20

de=e(j)-e(j-1)

fm=(f(j)+f(j-1))/2.

int=int+de*fm

20 continue

mr=exp(-int)

return

end

```

subroutine compres (pl,m1,t1)
implicit real (a-i,l-z)
logical tpctest
dimension mn1(5),mn2(5),m2(5),prat(5),trat(5)
COMMON/COMB/PCI,MCI,TCI,rci,vci,tpctest
open(unit=8,file='comp.dat')
data pi/3.14159/
j=0
g=1.4
pold=p1
mold=m1
told=t1
20 j=j+1
read(8,30) tet
30 format(f6.3)
tet=tet*pi/180.
call beta(m1,tet,b)
mn1(j)=m1*sin(b)
a=2.*g/(g-1)
mns=mn1(j)**2
mn2(j)=sqrt((mns+a/g)/(a*mns-1.))
m2(j)=mn2(j)/(sin(b-tet))
g1=g+1.0
prat(j)=1.0+2.0*g*(mns-1.0)/g1
drat=g1*mns/((g-1.0)*mns+2.0)
trat(j)=prat(j)/drat
if(j.lt.4) then
ml=m2(j)
tl=t1*trat(j)
pl=p1*prat(j)
goto 20
endif
pci=p1*prat(j)
tci=t1*trat(j)
mci=m2(j)
pl=pold
tl=told
ml=mold
tet=tet*180./pi
b=b*180./pi
rewind 8
return
end

```

c
c

```

subroutine beta(m1,t,b)
implicit real(a-i,l-z)

```

c

```

g=1.4
b=0.3
r=m1**2
p=tan(t)
10 x=sin(b)
y=cos(b)
f=r*p*g+r*p*cos(2.*b)+2.*p-2.*r*y*x+2.*y/x
fp=-2.*r*p*sin(2.*b)-2.*r*y**2+2.*r*x**2-2./x**2
bold=b
b=b-f/fp

```

```
_(abs((b-bold)/bold).gt.0.001) goto 10  
return  
end
```

```
C  
C  
SUBROUTINE DRAG (TETA,Q,VP,FD,m)
```

```
C  
IMPLICIT REAL (A-H,L-Z)
```

```
C  
C = 0.003703+0.03639/M+(0.003153+0.04251/M)*TETA*TAN(TETA)
```

```
C  
CALL LENGTH (VP,L,VB)
```

```
C  
SPL = 0.36 *L**2 +200.
```

```
FD = C* SPL * Q
```

```
RETURN
```

```
END
```

```
C  
C  
SUBROUTINE AINLET (rho,v,FT,IS,F,A,D)
```

```
C  
IMPLICIT REAL (A-I,L-Z)
```

```
logical tpstest
```

```
C  
COMMON/COMB/PCI,MCI,TCI,rci,vci,tpstest
```

```
COMMON PI
```

```
C  
AFR=FT/IS/(1.+F)
```

```
A = AFR/rho/V
```

```
D = SQRT(4.0*A/PI)
```

```
RETURN
```

```
END
```

```
C  
C  
SUBROUTINE LENGTH (VP,L,VB)
```

```
C  
REAL L
```

```
C  
VB=1.3*VP+250.
```

```
L=(VB/0.05)**(1./3.)
```

```
RETURN
```

```
END
```

SUBROUTINE TCALC

MAIN PROGRAM FOR THERMODYNAMIC CALCULATIONS

DOUBLE PRECISION G,X

```
REAL MIX(15)
INTEGER SPECE
INTEGER DATA, OMIT, ENSERT, REAC, BLANK, THRM, END, SUB
LOGICAL SHOCK, MMHG, UV, IC, DETN, SIUNIT, EUNITS, NSQM, CALCH
LOGICAL HP, SP, TP, NEWR, IONS, MOLES, FROZ, EQL, PSIA, RKT, VOL, TV, SV
LOGICAL FA, OF, ERATIO, FPCT, OTTO, HTEST, H, WRT, tptest
```

```
DIMENSION OMIT(3,3), NCD(4), ENSERT(3,3), RHO(26),
1 VL(26), DAT(22)
DIMENSION SPECE(2,3), TEMPR(20), TABLS(20,3)
```

COMMON SPECE , TEMPR , TABLS

```
COMMON /POINTS/HSUM(13), SSUM(13), CPR(13), DLVTP(13), DLVPT(13),
1 GAMMAS(13), P(26), T(52), V(13), PPP(13), WM(13), SONVEL(13), TTT(13),
2 VLM(13), TOTN(13)
COMMON /SPECES/COEF(2,7,150), S(150), HO(150), DELN(150), DUMMY(150),
1 EN(150,13), ENLN(150), A(10,150), SUB(150,3), IUSE(150), TEMP(50,2)
COMMON /MISC/ENN, SUMN, TT, SO, ATOM(3,101), LLMT(10), BO(10), BOP(10,2),
1 TM, TLOW, TMID, THIGH, PP, CPSUM, OF, EQRAT, FPCT, R, RR, HSUBO, AM(2),
2 HPP(2), RH(2), VMIN(2), VPLS(2), WP(2), DATA(22), NAME(15,5),
3 ANUM(15,5), PECWT(15), ENTH(15), FAZ(15), RTEMP(15), FOX(15), DENS(15),
4 RHOP, RMW(15), TLN, CR, OXF(15), ENNL, TRACE, LLMTS(10), SBOP(10,2)
COMMON /DOUBLE/ G(20,21), X(20)
COMMON /INDX/IDEBUG, CONVG, TP, HP, SP, ISV, NPP, MOLES, NP, NT, NPT, NLM,
1 NS, KMAT, IMAT, IQ1, IOF, NOF, NOMIT, IP, NEWR, NSUB, NSUP, RKT, DETN, SHOCK,
2 IONS, NC, NSERT, JSOL, JLIQ, KASE, NREAC, IC, JS1, VOL, IT, CALCH, NLS, LOGV,
3 ISUP, ISUB, ITNUM, ITM, INCDFZ, INCDEQ, CPRF, IPP, SEQL, PCPLT
COMMON /PERF/PCP(22), VMOC(13), SPIM(13), VACI(13), SUBAR(13),
1 SUPAR(13), APP(13), AEAT(13), CSTR, EQL, FROZ, SSO, AREA, AWT, NFZ,
2 APPL, ARATIO, ELN
COMMON/FLG/JPH1, HTEST, WRT, JQ
COMMON/COMB/PCI, MCI, TCI, rci, vci, tptest
COMMON/DNS/rhoce, pce, GAMAce, SVELce, OFRAT, hce, tce, cpce
```

```
EQUIVALENCE (OMIT, ENLN), (ENSERT, DELN), (OXF, MIX), (HTEST, H),
1 (OF, OXFL), (RHO, P, VL), (SO, SO), (OTTO, GPCVFR), (DATA, DAT)
```

```
DATA MIT/4HOMIT/, BLANK/1H /, REAC/4HREAC/, IZ/2HOO/,
1 NMLT/4HNAME/, IE/1HE/, INSERT/4HINSE/, THRM/4HTHER/, END/3HEND/,
2 GAS/1HG/, ND/4HLAST/
```

```
NAMELIST/INPT2/KASE, T, P, PSIA, MMHG, NSQM, V, RHO, ERATIO, OF, FPCT, FA,
1 MIX, TP, HP, SP, TV, UV, SV, RKT, SHOCK, DETN, OTTO, CR, SO, SO, IONS, IDEBUG,
2 TRACE, SIUNIT, EUNITS
```

NEWR = .FALSE.

```
1 RR = 8314.3
R = RR/4184.
```

```
203 IF(.NOT.H) GOTO 2035
READ (5,204) (DATA(I), I=1,15)
GOTO 2036
2035 READ (3,204) (DATA(I), I=1,15)
```

```
CONTINUE
FORMAT(5(3A4,3X))
IF(.NOT.WRT) GOTO 2046
WRITE (6,2045)(DATA(I),I=1,15)
2045 FORMAT(1X,5(3A4,3X))
2046 CONTINUE
IF(DATA(1).EQ.THRM) GOTO 90
IF(DATA(1).EQ.REAC) GOTO 11
IF (DATA(1).EQ.MIT) GOTO 205
IF (DATA(1).EQ.INSERT) GOTO 180
IF(DATA(1).EQ.NMLT) GOTO 210
IF(DATA(1).EQ.BLANK) GOTO 203
IF (DATA(1).EQ.END) GOTO 800
IF (DATA(1).EQ.ENDP) STOP
1023 WRITE(6,1024)
1024 FORMAT(40HOERROR IN ABOVE CARD.  CONTENTS IGNORED. )
GOTO 203
11 NSERT = 0
MOLES = .FALSE.
CALL REACT
IF(NLM.EQ.0) WRITE(6,52)
52 FORMAT(24HOERROR IN REACTANT CARDS)
CALCH = .FALSE.
DO 755 N=1,NREAC
IF(NAME(N,5).EQ.IZ) CALCH=.TRUE.
755 CONTINUE
GOTO 203
C
C READ THERMO AND TRANSPORT DATA FROM CARDS AND STORE ON TAPE 4
C
90 NEWR = .TRUE.
REWIND 4
IF (.NOT.H) GOTO 2037
READ(5,5) TLOW, TMID, THIGH
GOTO 2038
2037 READ(3,5) TLOW, TMID, THIGH
2038 CONTINUE
5 FORMAT (3F10.3)
IF(.NOT.WRT) GOTO 6
WRITE (4,5) TLOW, TMID, THIGH
6 IF(.NOT.H) GOTO 2039
97 READ (5,10)(DAT(I),I=1,16),NCD(1)
GOTO 2040
2039 READ (3,10)(DAT(I),I=1,16),NCD(1)
2040 CONTINUE
10 FORMAT(3A4,6X,2A3,4(A2,F3.0),A1,2F10.3,I15)
IF(DATA(1).EQ.BLANK) DATA(1)=END
IF(.NOT.WRT) GOTO 17
WRITE (4,10)(DAT(I),I=1,16)
17 IF(DATA(1).NE.END) GOTO 18
GOTO 203
18 READ(5,20)(DAT(I),I=1,5),NCD(2),(DAT(J),J=6,10),NCD(3),(DAT(K),
+K=11,14),NCD(4)
IF(.NOT.H) GOTO 2041
GOTO 2042
2041 READ(3,20)(DAT(I),I=1,5),NCD(2),(DAT(J),J=6,10),NCD(3),(DAT(K),
+K=11,14),NCD(4)
2042 CONTINUE
20 FORMAT(5E15.8,I5/5E15.8,I5/4E15.8,I20)
IF(.NOT.WRT) GOTO 26
```

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```
WRITE (4,21)(DAT(I),I=1,14)
FORMAT(5E15.8/5E15.8/4E15.8)
26 CONTINUE
DO 25 I=1,4
IF(NCD(I).EQ.I) GOTO 25
WRITE(6,22) (DATA(J),J=1,3)
22 FORMAT(28HOERROR IN ORDER OF CARDS FOR ,3A4)
25 CONTINUE
GOTO 97

C
C CHECK INSERT CARDS
C
180 DO 185 I=4,15,3
IF (DATA(I).EQ.BLANK) GOTO 185
NSERT = NSERT+1
ENSERT(1,NSERT) = DATA(I)
ENSERT(2,NSERT) = DATA(I+1)
ENSERT(3,NSERT) = DATA(I+2)
185 CONTINUE
GOTO 203

C
C CHECK OMIT CARDS
C
205 DO 208 I=4,15,3
IF(DATA(I).EQ.BLANK) GOTO 208
NOMIT = NOMIT+1
OMIT(1,NOMIT) = DATA(I)
OMIT(2,NOMIT) = DATA(I+1)
OMIT(3,NOMIT) = DATA(I+2)
208 CONTINUE
NEWNR= .TRUE.
REWIND 4
GOTO 203

C
C BEGIN NAMELIST INPT2
C
210 DO 299 I=1,26
P(I)= 0.
V(I) = 0.
299 CONTINUE
DO 306 I=1,52
T(I)=0.
306 CONTINUE
TRACE = 0.
S0 = 0.
V1 = 0.
V2 = 0.
CR = 0.
RHOP = 0.
PP=0.
TT=0.
KASE= 0
TP = .FALSE.
HP=.FALSE.
SP=.FALSE.
TV = .FALSE.
UV = .FALSE.
SV = .FALSE.
OTTO = .FALSE.
RKT = .FALSE.
```

ORIGINAL PAGE IS
OF POOR QUALITY

```
SHOCK = .FALSE.
DETN = .FALSE.
VOL = .FALSE.
MMHG = .FALSE.
PSIA = .FALSE.
NSQM = .FALSE.
SIUNIT = .FALSE.
EUNITS = .FALSE.
IONS = .FALSE.
IDEBUG = 0
FA= .FALSE.
OF= .FALSE.
ERATIO = .FALSE.
FPCT= .FALSE.
DO 303 I=1,15
MIX(I) = 0.
303 CONTINUE
NT = 1
EQL = .TRUE.
READ(1,1205)KASE,P(1),MIX(1),HP,NSQM,FA,ERATIO,IONS,SIUNIT
1205 FORMAT(I3,E12.6,F10.6,6L7)
REWIND 1
REWIND 5
REWIND 3
P(1)=PCI
if(tptest) then
t(1)=tci
tp=.true.
hp=.false.
endif
IF(.NOT.DETN.AND..NOT.SHOCK) GOTO 1303
DO 1300 N=1,NREAC
IF(FAZ(N).NE.GAS) GOTO 1301
1300 CONTINUE
GOTO 1303
1301 WRITE(6,1302)
1302 FORMAT(60HOCONDENSED REACTANTS NOT PERMITTED IN DETN OR SHOCK PROB
1LEMS)
GOTO 1
1303 IF(.NOT.TV.AND..NOT.UV.AND..NOT.SV) GOTO 304
VOL = .TRUE.
DO 1304 I=1,26
IF(RHO(I).NE.0.) VL(I) = 1./RHO(I)
IF(V(I).NE.0.) VL(I)=V(I)
IF(VL(I).EQ.0.) GOTO 1305
NP = I
1304 CONTINUE
1305 TP = TV
HP = UV
SP = SV
GOTO 322
304 DO 305 I=1,26
IF(P(I).EQ.0.) GOTO 322
NP = I
IF (MMHG) P(NP) = P(NP)/760.
IF(PSIA) P(NP)=P(NP)/14.696006
IF(NSQM) P(NP)=P(NP)/101325.
305 CONTINUE
322 DO 307 IS = 1,52
IF (T(IS).EQ.0.) GOTO 722
```

```
      I = IS  
      CONTINUE  
722 DO 625 IST=1,15  
      IF( MIX(IST).NE.0.) GOTO 323  
      IF(IST.NE.1) GOTO 745  
      WRITE(6,724)  
724 FORMAT(48HONO INPT2 VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT )  
      IF (WP(2).NE.0.) OXFL = WP(1)/WP(2)  
      GOTO 333  
323 OXFL = MIX(IST)  
      IF(FA) OXFL =1./MIX(IST)  
      IF(FPCT) OXFL =(100.-MIX(IST))/MIX(IST)  
      IF(.NOT.ERATIO) GOTO 333  
      EQRAT = MIX(IST)  
      IF(EQRAT.EQ.1.) EQRAT = 1.0000045  
      OXFL = (-EQRAT*VMIN(2)-VPLS(2))/(VPLS(1)+EQRAT*VMIN(1))
```

C
C
OFRAT=OXFL

```
333 OXF(IST) = OXFL  
      NOF = IST  
625 CONTINUE  
745 IF (.NOT.IONS) GOTO 746  
      IF(LLMT(NLM).EQ.IE) GOTO 746  
      NLM = NLM+1  
      IF(LLMT(NLM).NE.IE) NEWR=.TRUE.  
      REWIND 4  
      LLMT(NLM) = IE  
      BOP(NLM,1) = 0.  
      BOP(NLM,2) = 0.  
      GOTO 748  
746 IF(LLMT(NLM).NE.IE) GOTO 748  
      DO 747 J=1,NS  
      IF(A(NLM,J).NE.0.) IUSE(J)=-10000  
747 CONTINUE  
      NLM = NLM-1  
748 CONTINUE  
      IF(NEWR) CALL SEARCH  
      IF(NS.EQ.0) GOTO 1
```

C
C
C
INITIAL ESTIMATES

```
      S0 = S0/R  
      ENN = .1  
      ENNL = -2.3025851  
      SUMN = ENN  
      XI = NS - NC  
      XI = ENN/XI  
      XLN = ALOG(XI)  
      DO 432 J=1,NS  
      IF(IUSE(J).GT.0) IUSE(J)=-IUSE(J)  
      IF(IUSE(J).EQ.-10000.AND.IONS) IUSE(J) = 0  
      EN(J,1) = 0.  
      ENLN(J) = 0.  
      IF (IUSE(J).NE.0) GOTO 432  
      EN(J,1) = XI  
      ENLN(J) = XLN  
432 CONTINUE  
      IQ1 = NLM+1  
      IF (NC.EQ.0.OR.NSERT.EQ.0) GOTO 790
```



```

      J 302 I=1, NSERT
      INC = 0
      DO 301 J=1, NS
      IF(IUSE(J).EQ.0) GOTO 301
      INC = INC+1
      IF(SUB(J,1).NE.ENSERT(1,I)) GOTO 301
      IF(SUB(J,2).NE.ENSERT(2,I)) GOTO 301
      IF(SUB(J,3).NE.ENSERT(3,I)) GOTO 301
      IF(T(1).EQ.0.) GOTO 295
      IF(T(1).LT.TEMP(INC,1).OR.T(1).GT.TEMP(INC,2)) GOTO 301
295  IQ1 = IQ1+1
      IUSE(J)= -IUSE(J)
      GOTO 302
301  CONTINUE
302  CONTINUE
      NSERT = 0
790  CONTINUE
      IF(.NOT.TP.AND..NOT.HP.AND..NOT.SP) GOTO 791
      CALL THERMP
      GOTO 800
C
791  CONTINUE
C   IF(DETN) CALL DETON
C   IF(RKT) CALL ROCKET
C   IF(SHOCK) CALL SHCK
800  CONTINUE
      RETURN
      END
C
      SUBROUTINE REACT
C
      LOGICAL HP, SP, TP, CONVG, NEWR, IONS, MOLES, VOL, HTEST, WRT
C
      DIMENSION ANAME(15,5), V(10)
C
      COMMON /MISC/ENN, SUMN, TT, SO, ATOM(3,101), LLMT(10), BO(10), BOP(10,2),
1  TM, TLOW, TMID, THIGH, PP, CPSUM, OF, EQRAT, FPCT, R, RR, HSUBO, AM(2),
2  HPP(2), RH(2), VMIN(2), VPLS(2), WP(2), DATA(22), NAME(15,5),
3  ANUM(15,5), PECWT(15), ENTH(15), FAZ(15), RTEMP(15), FOX(15), DENS(15),
4  RHOP, RMW(15), TLN, CR, OXF(15), ENNL, TRACE, LLMTS(10), SBOP(10,2)
      COMMON /INDX/IDEBUG, CONVG, TP, HP, SP, ISV, NPP, MOLES, NP, NT, NPT, NLM,
1  NS, KMAT, IMAT, IQ1, IOF, NOF, NOMIT, IP, NEWR, NSUB, NSUP, RKT, DETN, SHOCK,
2  IONS, NC, NSERT, JSOL, JLIQ, KASE, NREAC, IC, JS1, VOL, IT, CALCH, NLS, LOGV,
3  ISUP, ISUB, ITNUM, ITM, INCDFZ, INCDEQ, CPRF, IPP, SEQL, PCPLT
      COMMON/FLG/JPH1, HTEST, WRT, JQ
      COMMON/COMB/PCI, MCI, TCI, rci, vci, tptest
C
      EQUIVALENCE (NAME, ANAME), (NLM, L), (BLANK, LANK)
C
      DATA MOL/1HM/, OX/1HO/, LANK/1H /, IZERO/2H00/, ZERO/1H0/
C
      DO 10 K=1, 2
      WP(K)=0.
      HPP(K)=0.
      RH(K)=0.
      VPLS(K)=0.
      VMIN(K)=0.
      AM(K)=0.
      DO 8 J=1, 10
      LLMT(J)=0
      BOP(J, K)=0.

```

```

CONTINUE
10 CONTINUE
NFUEL = 0
N=1
L=1

C
C READ AND WRITE REACTANT CARDS
C
20 CONTINUE
IF(.NOT.HTEST) GOTO 1022
READ(5,21) (NAME(N,I), ANUM(N,I), I=1,5), PECWT(N), MOLE, ENTH(N),
1 FAZ(N), RTEMP(N), FOX(N), DENS(N)
21 FORMAT(5(A2,F7.5), F7.5, A1, F9.5, A1, F8.5, A1, F8.5)
GOTO 1023
1022 READ(3,21) (NAME(N,I), ANUM(N,I), I=1,5), PECWT(N), MOLE, ENTH(N),
+ FAZ(N), RTEMP(N), FOX(N), DENS(N)
1023 CONTINUE
IF(NAME(N,1).EQ.LANK) GOTO 200
IF(L.EQ.0) GOTO 20
IF(.NOT.WRT) GOTO 35
WRITE (6,31) (NAME(N,I), ANUM(N,I), I=1,5), PECWT(N), MOLE, ENTH(N),
1 FAZ(N), RTEMP(N), FOX(N), DENS(N)
31 FORMAT(1X, 5(A2, 1X, F7.4, 2X), F8.4, 2X, A1, F11.2, 2X, A1, 2X, F8.3, 2X,
1 A1, 3X, F8.5)
35 IF(MOLE.EQ.MOL) MOLES=.TRUE.

C
C IF OXIDANT, K=1
C IF FUEL, K=2
C
IF(FOX(N).EQ.ZERO) FOX(N)=OX
K = 1
IF(FOX(N).EQ.OX) GOTO 37
K = 2
NFUEL = NFUEL+1
37 DO 38 J=1,15
DATA(J) = 0.
38 CONTINUE
RM=0.

C
C STORE ATOMIC SYMBOLS IN LLMT ARRAY.
C CALCULATE MOLECULAR WEIGHT.
C TEMPORARILY STORE ATOMIC VALENCE IN V.
C
DO 100 JJ=1,5
IF(ANUM(N,JJ).EQ.0.) GOTO 101
IF(ANAME(N,JJ).EQ.ZERO) ANAME(N,JJ)=OX
DO 41 J=1,10
NJ = J
IF(LLMT(J).EQ.0) GOTO 45
IF(NAME(N,JJ).EQ.LLMT(J)) GOTO 46
41 CONTINUE
45 L = NJ
LLMT(J)=NAME(N,JJ)
46 DO 48 KK=1,101
IF(ATOM(1, KK).EQ.ANAME(N,JJ)) GOTO 50
48 CONTINUE
L=L+1
GOTO 20
50 RM=RM+ANUM(N,JJ)*ATOM(2, KK)
V(J)=ATOM(3, KK)

```

```
DATA(J)=ANUM(N,JJ)
CONTINUE

C ADD CONTRIBUTIONS TO WP(K), HPP(K), AM(K), BOP(I,K) AND RH(K)
C
101 PCWT=PECWT(N)
    IF(MOLES) PCWT=PCWT*RM
    WP(K)=WP(K) + PCWT
    EM = ENTH(N)
    IF(NAME(N,5).NE.IZERO)HPP(K)=HPP(K)+EM*PCWT/(RM*R)
C WRITE(6,300) K,AM(K),PCWT,RM,N,NAME(N,5)
C 300 FORMAT(1H,'AM(',I1,')=' ,F7.3,'PCWT=' ,F7.3,'RM=' ,E12.6,
C &'NAME(',I3,',5)=' ,I5)
    AM(K)=AM(K)+PCWT/RM
    DO 110 J=1,L
    BOP(J,K)=DATA(J)*PCWT/RM +BOP(J,K)
110 CONTINUE
    IF(DENS(N).NE.0.)GOTO 115
    GOTO 117
115 RH(K)=RH(K)+PCWT/DENS(N)
117 RMW(N) = RM
    N = N+1
    IF(N.NE.16) GOTO 20
200 NREAC =N-1
    IF(NFUEL.GT.0) GOTO 210

C
C 100 PERCENT OXIDANT, CALL REACTANTS FUEL
C
DO 205 N=1,NREAC
FOX(N) = BLANK
205 CONTINUE
RH(2) = RH(1)
RH(1) = 0.
WP(2) = WP(1)
WP(1) = 0.
HPP(2) = HPP(1)
AM(2) = AM(1)
AM(1) = 0.
DO 208 J=1,L
BOP(J,2) = BOP(J,1)
208 CONTINUE
210 IF(L.EQ.0) GOTO 1000

C
C NORMALIZE HPP(K),AM(K),BOP(I,K), AND PECWT(N).
C CALCULATE RH(K), V+(K), AND V-(K)
C
DO 220 K=1,2
IF(WP(K).EQ.0.)GOTO 220
HPP(K)=HPP(K)/WP(K)
AM(K) = WP(K)/AM(K)
IF(RH(K).NE.0.)RH(K)=WP(K)/RH(K)
DO 215 J=1,L
BOP(J,K)=BOP(J,K)/WP(K)
IF(V(J).LT.0.)VMIN(K)= VMIN(K)+BOP(J,K)*V(J)
IF(V(J).GT.0.)VPLS(K)=VPLS(K)+BOP(J,K)*V(J)
215 CONTINUE
IF(MOLES) GOTO 220
DO 218 N=1,NREAC
IF(FOX(N).EQ.OX.AND.K.EQ.2) GOTO 218
IF(FOX(N).NE.OX.AND.K.EQ.1) GOTO 218
```

ECWT(N) = PECWT(N)/WP(K)
 200 CONTINUE
 220 CONTINUE
 NEWR=.TRUE.

C
 C ARE ELEMENTS SAME AS FOR LAST SET OF REACTANTS, IF SO, NEWR=.FALSE.
 C

IF(NLM.NE.NLS) GOTO 226
 IF(NOMIT.NE.0) GOTO 226
 DO 224 I=1,NLS
 DO 222 J=1,NLM
 IF(LLMT(J).NE.LLMTS(I)) GOTO 222
 SBOP(I,1) = BOP(J,1)
 SBOP(I,2) = BOP(J,2)
 GOTO 224
 222 CONTINUE
 GOTO 226
 224 CONTINUE
 NEWR = .FALSE.
 DO 225 I=1,NLM
 LLMT(I) = LLMTS(I)
 BOP(I,1) = SBOP(I,1)
 BOP(I,2) = SBOP(I,2)
 225 CONTINUE
 GOTO 229

C
 C
 226 NLS = NLM
 NOMIT = 0
 REWIND 4
 DO 228 I=1,NLM
 LLMTS(I) = LLMT(I)
 228 CONTINUE
 229 DO 230 N=1,NREAC
 IF (DENS(N).NE.0.) GOTO 230
 RH(2) = 0.
 RH (1) = 0.
 GOTO 1000
 230 CONTINUE
 1000 RETURN
 END

C
 C SUBROUTINE HCALC

C
 C CALCULATE PROPERTIES FOR TOTAL REACTANT USING THERMO DATA FOR
 C ONE OR MORE REACTANTS.

C
 C THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR
 C IBM 360 MACHINES ONLY

C
 C DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS
 C DOUBLE PRECISION COEF,S,EN,ENLN,HO,DELN

C
 C LOGICAL MOLES,VOL,SHOCK,CALCH
 C CALCULATE ENTHALPY FOR PROPELLANT USING COEFFICIENTS
 C DIMENSION NUM(15,5)

C
 C COMMON /POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),
 C 1 GAMMAS(13),P(26),T(52),V(13),PPP(13),WM(13),SONVEL(13),TTT(13),
 C 2 VLM(13),TOTN(13)

```
COMMON /SPECES/COEF(2,7,150),S(150),HO(150),DELN(150),DUMMY(150),  
1 EN(150,13),ENLN(150),A(10,150),SUB(150,3),IUSE(150),TEMP(50,2)  
COMMON /MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(10),B0(10),BOP(10,2),  
1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),  
2 HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),  
3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),  
4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)  
COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,  
1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEWNR,NSUB,NSUP,RKT,DETN,SHOCK,  
2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,IT,CALCH,NLS,LOGV,  
3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQL,PCPLT
```

```
C  
EQUIVALENCE (ANUM,NUM),(L,NLM),(J,JS1)  
EQUIVALENCE (AM1,DATA(20)),(CPR1,DATA(21))
```

```
C  
DATA AG/1HG/,IZERO/2H00/,OX/1HO/,BLK/1H /
```

```
C  
TSAVE = TT
```

```
C  
CALCUALTE MOLECULAR WEIGHT OF TOTAL REACTANT, AM1.
```

```
C  
IF (AM(1).NE.0.0 .AND. AM(2).NE.0.0) GOTO 4  
AM1= AM(2)  
IF (AM(2).EQ.0.0) AM1= AM(1)  
GOTO 9  
4 AM1=(OF+1.)*AM(1)*AM(2)/(AM(1)+OF*AM(2))  
9 TM = 0.  
IF(PP.GT.0.) TM = ALOG(PP*AM1)  
SSUM(NPT) = 0.  
HPP(1) = 0.  
HPP(2) = 0.  
HSUBO = 0.  
CPR1 = 0.  
ANN = (1.+OF)
```

```
C  
LOOP ON REACTANTS.
```

```
C  
IF OXIDANT, K=1
```

```
C  
IF FUEL, K=2
```

```
C  
DO 900 N=1,NREAC
```

```
K=2
```

```
IF(FOX(N).EQ.OX)K=1
```

```
IF(NAME(N,5).NE.IZERO) GOTO 90
```

```
IF(.NOT.CALCH.AND.TT.NE.0.) GOTO 15
```

```
TT = RTEMP(N)
```

```
C  
IS TT IN RANGE
```

```
C  
15 IF(SHOCK) GOTO 16
```

```
IF(TT.LT.(TLOW/1.2).OR.TT.GT.(THIGH*1.2)) GOTO 75
```

```
C  
16 J = NUM(N,5)
```

```
IF (J.NE.0) GOTO 90
```

```
DO 10 M=1,L
```

```
DATA(M)=0.
```

```
10 CONTINUE
```

```
C  
TEMPORARILY STORE STOICHIOMETRIC COEFFICIENTS IN DATA ARRAY.
```

```
C  
DO 40 I=1,4
```

```
IF(ANUM(N,I).EQ.0.)GOTO 50
```

```
      J 20 M=1,L
      IF(LLMT(M).EQ.NAME(N,I)) GOTO 30
20 CONTINUE
30 DATA(M)=ANUM(N,I)
40 CONTINUE
50 IS=0

C
C SEARCH FOR REACTANT IN THERMO SPECIES. STORE INDEX IN NUM(N,5).
C

      DO 70 M=1,NS
      J=M
      IF(IUSE(J).EQ.0)GOTO 55
      IS = IS+1
      IF(FAZ(N).EQ.AG)GOTO 70
      IF(TT.GT.TEMP(IS,2).AND.TEMP(IS,2).NE.THIGH) GOTO 70
      IF(TT.LT.TEMP(IS,1).AND.TEMP(IS,1).NE.TLOW) GOTO 70
      GOTO 56
55 IF(FAZ(N).NE.AG.AND.FAZ(N).NE.BLK) GOTO 70
56 DO 60 I=1,L
      IF(A(I,J).NE.DATA(I)) GOTO 70
60 CONTINUE
      NUM(N,5) = J
      GOTO 90
70 CONTINUE
      GOTO 80

C
C CALCULATE EN FOR REACTANT AND CALL CPHS TO CALCULATE PROPERTIES.
C

90 IF (MOLES) ENJ = PECWT(N)/WP(K)
      IF (.NOT.MOLES) ENJ = PECWT(N)/RMW(N)
      ENJ = ENJ/ANN
      IF(K.EQ.1) ENJ = ENJ*OF
      IF(NAME(N,5).NE.IZERO)GOTO 500
      NSS = NS
      NS = J
      TLN = ALOG(TT)
      IF(.NOT.CALCH) EN(J,NPT) = ENJ
      CALL CPHS
      NS = NSS
      IF (HO(J).GT..01 .AND. HO(J).LT..01) HO(J) = 0.
      RTEMP(N) = TT
      IF(VOL) HO(J)=HO(J)-1.
      ENTH(N) = HO(J)*R*TT

C
C ADD CONTRIBUTION TO CP, H, AND S OF TOTAL REACTANT.
C

      CPR1 = CPR1 + CPSUM
      SSUM(NPT) = SSUM(NPT) + ENJ * (S(J)-ALOG(ENJ)-TM)
500 ER = ENTH(N)*ENJ/R
      HSUB0 = HSUB0+ER
      HPP(K) = HPP(K)+ER
900 CONTINUE
      IF(TSAVE.NE.0.) TT=TSAVE
      GOTO 1000
75 WRITE(6,76)
76 FORMAT(50HOREACTANT TEMPERATURE OUT OF RANGE OF THERMO DATA )
      TT = 0.
      GOTO 1000
80 WRITE(6,85) N
85 FORMAT(9HOREACTANT,I2,22H IS NOT IN THERMO DATA )
```

```
      I = 0.  
      RETURN  
      END
```

```
C  
      SUBROUTINE EQLBRM
```

```
C ROUTINE TO CALCULATE EQUILIBRIUM COMPOSITION AND PROPERTIES
```

```
C  
      DOUBLE PRECISION X,G,SUM  
      DOUBLE PRECISION TND
```

```
C  
C THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR  
C IBM 360 MACHINES ONLY
```

```
C  
C DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS  
C DOUBLE PRECISION COEF,S,EN,ENLN,HO,DELN  
C DOUBLE PRECISION ENL,PROW,DLNT,AA
```

```
C  
C LOGICAL HP,SP,TP,CONVG,IONS,SINGC,LOGV,ISING,IC,VOL,SHOCK,RITE  
C LOGICAL WRT
```

```
C  
      COMMON /POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),  
1 GAMMAS(13),P(26),T(52),V(13),PPP(13),WM(13),SONVEL(13),TTT(13),  
2 VLM(13),TOTN(13)  
      COMMON /SPECES/COEF(2,7,150),S(150),HO(150),DELN(150),DUMMY(150),  
1 EN(150,13),ENLN(150),A(10,150),SUB(150,3),IUSE(150),TEMP(50,2)  
      COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),  
1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),  
2 HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),  
3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),  
4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)  
      COMMON /DOUBLE/ G(20,21), X(20)  
      COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,  
1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEW,NSUB,NSUP,RKT,DETN,SHOCK,  
2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,IT,CALCH,NLS,LOGV,  
3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQ,PCPLT  
      COMMON/FLG/JPH1,HTEST,WRT,JQ
```

```
C  
      EQUIVALENCE (NLM,L)
```

```
C  
      DATA IE/1HE/,SMALNO/1.E-6/,SMNOL/-13.815511/,ITN/100/
```

```
C  
      E = 2.718281828459  
      SINGC = .FALSE.  
      ENL = ENNL  
      RITE = .FALSE.  
      IF(IDEBUG.GT.0.AND.NPT.GE.IDEBUG) RITE=.TRUE.  
      SIZE = 18.420681  
      ISING = .FALSE.  
      LOGV = .FALSE.  
      IF(.NOT.VOL) GOTO 6  
      RV = RR/101.325  
      PP = RV*ENN*TT/VLM(NPT)
```

```
6 TLN = ALOG(TT)  
      CONVG = .FALSE.  
      ITNUMB = ITN  
      JS1 = 1  
      CALL CPHS  
      TM = ALOG(PP/ENN)
```

```
C  
      IF (.NOT.IONS.OR.IE.EQ.LLMT(L)) GOTO 33
```

```
      = L+1
      IQ1 = IQ1+1
      DO 499 J = 1, NS
      IF (A(L, J) .EQ. 0.) GOTO 499
      EN(J, NPT) = 1.E-8
      ENLN(J) = -SIZE
      IUSE(J) = 0
499 CONTINUE
      33 IF(.NOT.WRT) GOTO 43
      IF(NPT.EQ.1.AND..NOT.SHOCK) WRITE(6, 244) (LLMT(I), I=1, L)
      244 FORMAT (4HOPT ,14(5X,A4))
C
C      BEGIN ITERATION
C
      43 IF (.NOT.CONVG) GOTO 62
      SUMN = ENN
      IF(JSOL.EQ.0) GOTO 62
      ENSOL = EN(JSOL, NPT)
      EN(JSOL, NPT) = EN(JSOL, NPT)+EN(JLIQ, NPT)
      IUSE(JLIQ) = -IUSE(JLIQ)
      IQ1 = IQ1-1
      DLVTP(NPT) = 0.
      CPR(NPT) = 0.
      GAMMAS(NPT) = 0.
      LOGV = .TRUE.
      62 CALL MATRIX
      NUMB = ITN-ITNUMB+1
      IQ2 = IQ1 + 1
      IF(CONVG) IMAT=IMAT-1
      IF(.NOT.RITE) GOTO 72
      IF(.NOT.CONVG) GOTO 88
      IF(.NOT.WRT) GOTO 83
      IF(.NOT.LOGV) WRITE(6, 81)
      81 FORMAT(15HOT DERIV MATRIX)
      IF(LOGV) WRITE(6, 82)
      82 FORMAT(15HOP DERIV MATRIX)
      83 CONTINUE
      GOTO 89
      88 IF(.NOT.WRT) GOTO 89
      WRITE(6, 772) NUMB
      772 FORMAT (11HOITERATION ,I3,6X,7HMATRIX //)
      89 CONTINUE
      IF(.NOT.WRT) GOTO 72
      DO 911 I=1, IMAT
      911 WRITE (6, 73) (G(I, K), K=1, KMAT)
      72 ITST = IMAT
      CALL GAUSS
      IF(ITST.NE.IMAT) GOTO 774
      IF(.NOT.RITE) GOTO 773
      WRITE (6, 373) (LLMT(I), I=1, L)
      373 FORMAT (7HOPI ,9(A4,10X))
      WRITE (6, 73) (X(I), I=1, IMAT)
      73 FORMAT (9E14.6)
      773 IF(.NOT.CONVG) GOTO 85
      IF(.NOT.LOGV) GOTO 174
      GOTO 171
C
C      TEMPERATURE DERIVATIVES--CONVG=T, LOGV=F
C
      174 DLVTP(NPT) = 1.-X(IQ1)
```



```
      R(NPT) = G(IQ2,IQ2)
      DO 176 J=1,IQ1
      CPR(NPT) = CPR(NPT)-G(IQ2,J)*X(J)
176 CONTINUE
C
C   PRESSURE DERIVATIVE--CONVG=T, LOGV=T
C
      LOGV = .TRUE.
      GOTO 62
C
C   SINGULAR MATRIX
C
774 IF(.NOT.CONVG) GOTO 775
      WRITE(6,172)
172 FORMAT(28HODERIVATIVE MATRIX SINGULAR )
      GOTO 1171
775 IF(.NOT.HP.OR.NPT.NE.1.OR.NC.EQ.0.OR.TT.GT.100.) GOTO 871
      WRITE(6,874)
874 FORMAT(96HLOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE
1BEEN INCLUDED ON AN INSERT CARD, RESTART )
      GOTO 873
871 WRITE(6,74)
      74 FORMAT(16HOSINGULAR MATRIX)
      IF(SINGC) GOTO 873
      DO 970 JJ = 1,NS
      IF(IUSE(JJ).NE.0) GOTO 970
      IF(EN(JJ,NPT).NE.0.) GOTO 970
      EN(JJ,NPT) = SMALNO
      ENLN(JJ) = SMNOL
970 CONTINUE
      IF(ISING) GOTO 870
      ISING = .TRUE.
      WRITE (6,776)
776 FORMAT (8HORESTART)
      GOTO 62
C
C   TEST FOR SINGULARITY TO CONDENSED SPECIES.
C
870 NCOND = IQ1-NLM-1
      IF(NCOND.LT.2.OR.SIZEG.EQ.0.) GOTO 873
      DO 872 J=1,NS
      IF(IUSE(J).LE.0) GOTO 872
      IF(J.EQ.JDELG) GOTO 872
      DO 671 I=1,NLM
      IF(A(I,J).EQ.A(I,JDELG)) GOTO 671
      IF(A(I,J).EQ.0..OR.A(I,JDELG).EQ.0.) GOTO 872
671 CONTINUE
      SINGC = .TRUE.
      IQ1 = IQ1-1
      EN(J,NPT) = 0.
      IUSE(J) = -IUSE(J)
872 CONTINUE
      IF(SINGC) GOTO 40
      GOTO 873
C
C   OBTAIN CORRECTIONS TO THE ESTIMATES
C
85 ITNUMB= ITNUMB-1
      KK = L + 1
      IF(VOL) X(IQ2)=X(IQ1)
```

```

-r(TP) X(IQ2)=0.
DLNT= X(IQ2)
SUM = X(IQ1)
IF(.NOT.VOL) GOTO 97
X(IQ1) = 0.
SUM = -DLNT
97 DO 101 J=1,NS
IF (IUSE(J)) 101,98,100
98 DELN(J) = HO(J)*DLNT-HO(J)+S(J)-ENLN(J)-TM+SUM
DO 99 K=1,L
DELN(J)= DELN(J)+A(K,J)*X(K)
99 CONTINUE
GOTO 101
100 DELN(J) = X(KK)
KK = KK + 1
101 CONTINUE
C
C CALCULATE CONTROL FACTOR,AMBDA
C
AMBDA= 1.
AMBDA1= 1.
SUM = X(IQ1)
IF(SUM.LT.0.) SUM=-SUM
IF(DLNT.GT.SUM) SUM=DLNT
IF(-DLNT.GT.SUM) SUM=-DLNT
DO 917 J=1,NS
IF (IUSE(J).NE.0) GOTO 917
IF((EN(J,NPT).GT.0.) .AND. DELN(J).GT.SUM) SUM = DELN(J)
IF((EN(J,NPT).NE.0.) .OR. DELN(J).LE.0.) GOTO 917
SUM1 = (-9.212-ENLN(J)+ ENL)/(DELN(J)-X(IQ1))
IF(SUM1.LT.0.) SUM1=-SUM1
IF (SUM1.LT.AMBDA1) AMBDA1 = SUM1
917 CONTINUE
IF(SUM.GT.2.)AMBDA=2./SUM
IF (AMBDA1.LT.AMBDA) AMBDA = AMBDA1
IF(.NOT.RITE) GOTO 111
C
C INTERMEDIATE OUTPUT
C
WRITE(6,923) TT,ENN, ENL,PP,TM,AMBDA
923 FORMAT (3HOT=,E15.8,6H ENN=,E15.8,6H ENNL=,E15.8,5H PP=,E15.8,
1 9H LN P/N=,E15.8,8H AMBDA=,E15.8 )
IF(VOL) WRITE(6,1924) VLM(NPT)
1924 FORMAT(8H VOLUME=,E15.8,4HCC/G)
WRITE (6,924)
924 FORMAT(1H0,18X,2HNJ,12X,5HLN NJ,8X,9HDEL LN NJ,9X,6HHOJ/RT,9X,5HSO
1J/R,10X,7H-GQJ/RT,8X,6H-GJ/RT )
DO 926 J=1,NS
GNEG1 = S(J)-HO(J)
GNEG2 = GNEG1
IF(IUSE(J).EQ.0) GNEG2=GNEG2-ENLN(J)-TM
WRITE (6,925) SUB(J,1),SUB(J,2),
1SUB(J,3),EN(J,NPT),ENLN(J),DELN(J),HO(J),S(J),GNEG1,GNEG2
925 FORMAT (1X,3A4,7E15.6)
926 CONTINUE
IF(.NOT.WRT) GOTO 111
WRITE (6,110)
110 FORMAT(1H0)
C
C APPLY CORRECTIONS TO ESTIMATES

```

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```
1 SUM = 0.  
DO 113 J=1,NS  
IF (IUSE(J)) 113,112,114  
112 ENLN(J)=ENLN(J)+AMBDA*DELN(J)  
EN(J,NPT) = 0.  
IF((ENLN(J)- ENL+SIZE).LE.0.) GOTO 113  
EN(J,NPT) = E**ENLN(J)  
SUM = SUM+EN(J,NPT)  
GOTO 113  
114 EN(J,NPT) = EN(J,NPT) + AMBDA * DELN(J)  
113 CONTINUE  
SUMN = SUM  
IF (TP) GOTO 115  
TLN= TLN+AMBDA*DLNT  
TT = EXP(TLN)  
JS1 = 1  
CALL CPHS  
115 IF(VOL) GOTO 2115  
ENL = ENL+AMBDA*X(IQ1)  
ENN = E**ENL  
GOTO 1115  
2115 ENN = SUMN  
ENL = ALOG(ENN)  
PP = RV*TT*ENN/VLM(NPT)  
1115 TM = ALOG(PP/ENN)  
IF (LLMT(L).NE.IE) GOTO 116
```

C
C
C

```
DO 1116 J = 1,NS  
IF (A(L,J).EQ.0.) GOTO 1116  
IF (EN(J,NPT).GT.0.) GOTO 116  
1116 CONTINUE  
DO 1118 J=1,NS  
IF(A(L,J).NE.0.) IUSE(J) = -10000  
1118 CONTINUE  
L = L-1  
IQ1 = IQ1-1  
GOTO 43
```

C
C
C

```
116 IF (ITNUMB.EQ.0) GOTO 14  
IF (AMBDA.LT.1.) GOTO 43  
SUM = (ENN-SUMN)/ENN  
IF (SUM.LT.0.) SUM = -SUM  
IF (SUM.GT.0.5E-5) GOTO 43  
DO 130 J=1,NS  
IF (IUSE(J).LT.0) GOTO 130  
AA= DELN(J)/SUMN  
IF(AA.LT.0.) AA=-AA  
IF (IUSE(J).EQ.0) AA = AA*EN(J,NPT)  
IF(AA.GT.0.5E-5) GOTO 43  
130 CONTINUE
```

C
C
C

CALCULATE ENTROPY, CHECK ON DELTA S FOR SP PROBLEMS

```
TOTN(NPT) = 0.  
SSUM(NPT) = 0.
```

```
      J 183 J=1,NS
      IF(IUSE(J).LT.0) GOTO 183
      TOTN(NPT) = TOTN(NPT) + EN(J,NPT)
      SS = S(J)
      IF(IUSE(J).EQ.0) SS=SS-ENLN(J)-TM
      SSUM(NPT) = SSUM(NPT)+SS*EN(J,NPT)
183  CONTINUE
      IF(.NOT.SP.OR.NPT.EQ.1) GOTO 13
      SS = SSUM(NPT) -S0
      IF(SS.LT.(-0.00005).OR.SS.GT.0.00005) GOTO 43
      IF(RITE) WRITE(6,1183) SS
1183 FORMAT(12HODELTA S/R =,E15.8)
C
      13 CONVG= .TRUE.
      GOTO 160
      14 WRITE(6,973) ITN,NPT
      973 FORMAT(1HL,I2,69H ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREME
      INTS FOR THE POINT      ,I5)
      IF (.NOT.HP.OR.NPT.NE.1.OR.NC.EQ.0.OR.TT.GT.100.) GOTO 873
      WRITE(6,874)
      GOTO 873
C
C      CONVERGENCE TESTS ARE SATISFIED, TEST CONDENSED SPECIES.
C
      160 IF(NC.EQ.0) GOTO 143
      DO 146 J=1,NS
      IF(EN(J,NPT).GE.0.) GOTO 146
      IF (J.NE.JSOL .AND. J .NE.JLIQ) GOTO 147
      JSOL = 0
      JLIQ = 0
      147 IQ1 = IQ1 - 1
      EN(J,NPT) = 0.
      GOTO 166
      146 CONTINUE
      SIZEG = 0.
      INC = 0
      DO 170 J = 1,NS
      IF (IUSE(J).EQ.0 .OR. IUSE(J).EQ.-10000) GOTO 170
      INC = INC + 1
      IF(RITE) WRITE(6,144)(SUB(J,I),I=1,3),TEMP(INC,1),TEMP(INC,2),IUS
      1E(J),EN(J,NPT)
      144 FORMAT (1H0,3A4,2F10.3,3X,5HIUSE=,I4,E15.7)
      IF(EN(J,NPT).GT.0.) GOTO 169
      KG = 1
      IF(IUSE(J).EQ.-IUSE(J+1)) GOTO 154
      IF(J.EQ.1.OR.IUSE(J).NE.-IUSE(J-1)) GOTO 153
      KG = -1
      154 JKG = J + KG
      TMELT = TEMP(INC,1)
      IMP = INC + KG
      IF(TMELT.EQ.TEMP(IMP,2)) GOTO 158
      TMELT = TEMP(INC,2)
      IF (TMELT.EQ.TEMP(IMP,1)) GOTO 157
      WRITE (6,156)
      156 FORMAT (50H03 PHASES OF A CONDENSED SPECIES ARE OUT OF ORDER )
      GOTO 873
C
C      JTH SPECIES A SOLID (EN=0), (J+KG)TH SPECIES A LIQUID (EN IS +)
C
      157 IF(TT.GT.TMELT) GOTO 169
```

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```
IF (TP.AND.TT.EQ.TMELT) GOTO 169  
IF (TP) GOTO 1165  
IF (TT.LE.TMELT-150.) GOTO 1165  
JSOL = J  
JLIQ = JKG  
GOTO 159
```

```
C  
C JTH SPECIES A LIQUID(EN=0), (J+KG)TH SPECIES A SOLID (EN IS +)
```

```
C  
158 IF (TT.LT.TMELT) GOTO 169  
IF (TP.AND.TT.EQ.TMELT) GOTO 169  
IF (TP) GOTO 1165  
IF (TT.GE.TMELT+150.) GOTO 1165  
JSOL = JKG  
JLIQ = J  
159 TLN = ALOG (TMELT)  
TT = TMELT  
EN(JKG,NPT) = .5 * EN(JKG,NPT)  
EN(J,NPT) = EN(JKG,NPT)  
GOTO 165
```

```
C  
C WRONG PHASE INCLUDED FOR T INTERVAL, SWITCH EN
```

```
C  
1165 EN(J,NPT) = EN (JKG, NPT)  
IUSE(J) = -IUSE(J)  
IUSE (JKG) = -IUSE(JKG)  
EN(JKG,NPT)= 0.  
GOTO 40
```

```
153 IF (TT.LT.TEMP(INC,1) .AND.TEMP(INC,1).NE.TLOW) GOTO 169  
IF (TT.GT.TEMP(INC,2)) GOTO 169
```

```
C  
SUM = 0.  
DO 167 I = 1,L  
SUM = SUM + A(I,J)*X(I)  
167 CONTINUE  
DELG = H0(J)-S(J)-SUM  
IF(RITE) WRITE(6,168)DELG,SIZEG  
168 FORMAT (18H GO-SUM(AIJ*PII) =,E15.7,10X,17HMAX NEG DELTA G =,  
& E15.7)  
IF(DELG.GE.SIZEG .OR. DELG.GE.0.) GOTO 169  
SIZEG = DELG  
JDELG = J  
169 IF(INC.EQ.NC) GOTO 1160  
170 CONTINUE  
1160 IF (SIZEG.EQ.0.) GOTO 143  
J = JDELG  
165 IQ1 = IQ1 + 1  
166 IUSE(J) = - IUSE(J)  
40 CONVG = .FALSE.  
JS1 = 1  
CALL CPHS  
143 TN = NUMB  
TND = TN  
IF(.NOT.WRT) GOTO 2046  
IF(.NOT.SHOCK) WRITE(6,771)NPT,(X(IL),IL=1,L),TND  
771 FORMAT (I3,14D9.2)  
2046 CONTINUE  
JS1 = 1  
IF(TP.AND.CONVG) CALL CPHS  
ITNUMB = ITN
```

CALCULATE EQUILIBRIUM PROPERTIES

```

C
C
1171 DLVPT(NPT) = -1.
    DLVTP(NPT) = 1.
    CPR(NPT) = CPSUM
    GOTO 199

171 DLVPT(NPT) = -1. + X(IQ1)
    IF(JLIQ.EQ.0) GOTO 199
    EN(JSOL,NPT) = ENSOL
    IUSE(JLIQ) = -IUSE(JLIQ)
    HSUM(NPT) = HSUM(NPT)+EN(JLIQ,NPT)*(HO(JLIQ)-HO(JSOL))
    IQ1 = IQ1+1
    GAMMAS(NPT) = -1./DLVPT(NPT)
    GOTO 186

199 GAMMAS(NPT) = -1./(DLVPT(NPT)+(DLVTP(NPT)**2)*ENN/CPR(NPT))
186 TTT(NPT) = TT
    ENNL = ENL
    PPP(NPT) = PP
    VLM(NPT) = RR*ENN*TT/(101.325*PP)
    HSUM(NPT) = HSUM(NPT)*TT
    WM(NPT) = 1./ENN
    IF(TRACE.EQ.0.) GOTO 200
    DO 1200 J=1,NS
    IF(IUSE(J).NE.0) GOTO 1200
    IF(ENLN(J).GT.-87.) EN(J,NPT)=EXP(ENLN(J))
1200 CONTINUE
200 IF(.NOT.RITE) GOTO 863
    WRITE(6,201) NPT,PP,TT,HSUM(NPT),SSUM(NPT),WM(NPT),CPR(NPT),
1 DLVPT(NPT),DLVTP(NPT),GAMMAS(NPT),VLM(NPT)
201 FORMAT (7HOPOINT=,I3,3X,2HP=,E13.6,3X,2HT=,E13.6,3X,4HH/R=,E13.6
1,3X,4HS/R=,E13.6//3X,3HMW=,E13.6,3X,5HCP/R=,E13.6,3X,6HDLVPT=,
2E13.6,3X,6HDLVTP=,E13.6,3X,9HGAMMA(S)=,E13.6,3X,2HV=,E13.6)
863 IF(TT.GE.TLOW.AND.TT.LE.THIGH.OR.SHOCK) GOTO 1000
    WRITE(6,306) TT,NPT
306 FORMAT(17HOTHE TEMPERATURE=,E12.4,26H IS OUT OF RANGE FOR POINT,
& I5)
    IF(TT.GE.TLOW/1.5.AND.TT.LE.THIGH*1.25) GOTO 1000
    NPT = NPT+1

```

```

C
C ERROR, SET TT=0
C

```

```

873 TT=0.
    NPT = NPT-1
1000 RETURN
    END

```

```

C
C
C SUBROUTINE GAUSS
C
C SOLVE ANY LINEAR SET OF UP TO 20 EQUATIONS
C NUMBER OF EQUATIONS = IMAT
C
C DOUBLE PRECISION G,X,COEFX(20),SUM,Z

```

```

C
COMMON/DOUBLE/G(20,21),X(20)
COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,

```

NS, KMAT, IMAT, IQ1, IOF, NOF, NOMIT, IP, NEWR, NSUB, NSUP, RKT, DETN, SHOCK,
2 IONS, NC, NSERT, JSOL, JLIQ, KASE, NREAC, IC, JS1, VOL, IT, CALCH, NLS, LOGV,
3 ISUP, ISUB, ITNUM, ITM, INCDFZ, INCDEQ, CPRF, IPP, SEQL, PCPLT

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C
C DATA BIGNO/1.E+38/
C

C BEGIN ELIMINATION OF NTH VARIABLE
C

IUSE1 = IMAT+1

6 DO 45 NN=1, IMAT
IF(NN-IMAT) 8, 83, 8
83 IF(G(NN, NN)) 31, 23, 31

C SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW
C

8 DO 18 I=NN, IMAT
COEFX(I) = BIGNO
IF(G(I, NN).EQ.0.) GOTO 18
COEFX(I) = 0.
DO 10 J=NN, IUSE1
SUM = G(I, J)
IF(SUM.LT.0.) SUM=-SUM
IF(J.NE.NN) GOTO 9
Z = SUM
GOTO 10
9 IF(SUM.GT.COEFX(I)) COEFX(I)=SUM
10 CONTINUE
COEFX(I) = COEFX(I)/Z
18 CONTINUE

C LOCATE ROW WITH SMALLEST MAXIMUM COEFFICIENT
C

TEMP = BIGNO
I=0
20 DO 22 J=NN, IMAT
IF (COEFX(J)-TEMP) 87, 22, 22
87 TEMP=COEFX(J)
I=J
22 CONTINUE
IF(I) 28, 23, 28

C INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NTH
C VARIABLE FROM THE REMAINING EQUATIONS
C

C INTERCHANGE EQUATIONS I AND NN
C

28 IF(NN-I) 29, 31, 29
29 DO 30 J=NN, IUSE1
Z=G(I, J)
G(I, J)=G(NN, J)
G(NN, J)=Z
30 CONTINUE

C DIVIDE NTH ROW BY NTH DIAGONAL ELEMENT AND ELIMINATE THE NTH
C VARIABLE FROM THE REMAINING EQUATIONS
C

31 K = NN + 1
DO 36 J = K, IUSE1
IF(G(NN, NN).EQ.0.) GOTO 23
G(NN, J) = G(NN, J) / G(NN, NN)

CONTINUE
 IF(K-IUSE1) 88,45,88
 88 DO 44 I=K,IMAT
 40 DO 44 J = K,IUSE1
 G(I,J) = G(I,J) - G(I,NN)*G(NN,J)
 44 CONTINUE
 45 CONTINUE

C
 C BACKSOLVE FOR THE VARIABLES
 C

K = IMAT
 47 J = K + 1
 X(K) = 0.0DO
 SUM = 0.0
 IF(IMAT-J) 51,48,48
 48 DO 50 I=J,IMAT
 SUM = SUM + G(K,I)* X(I)
 50 CONTINUE
 51 X(K) = G(K,IUSE1) - SUM
 K = K - 1
 IF(K) 47,151,47
 23 IMAT = IMAT-1
 151 RETURN
 END

C
 C BLOCK DATA
 C

COMMON /MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(10),B0(10),BOP(10,2),
 1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AM(2),
 2 HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),
 3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),
 4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)
 COMMON /OUP/T/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4),
 1 FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMT19,FA1,FA2,
 2 FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0

C
 C ATOMIC SYMBOLS, WEIGHTS, AND VALENCES
 C

DATA ((ATOM(I,J),I=1,3),J=1,52)/ 2HE ,5.48597E-4,-1.,
 A 2HH , 1.00797 , 1., 2HHE, 4.0026, 0., 2HLI, 6.939 , 1.,
 B 2HBE, 9.0122 , 2., 2HB , 10.811 , 3., 2HC , 12.01115, 4.,
 C 2HN , 14.0067 , 0., 2HO , 15.9994,-2., 2HF , 18.9984 , -1.,
 D 2HNE, 20.183 , 0., 2HNA, 22.9898, 1., 2HMG, 24.312 , 2.,
 E 2HAL, 26.9815 , 3., 2HSI, 28.086 , 4., 2HP , 30.9738 , 5.,
 F 2HS , 32.064 , 4., 2HCL, 35.453 , -1., 2HAR, 39.948 , 0.,
 G 2HK , 39.102 , 1., 2HCA, 40.080 , 2., 2HSC, 44.956 , 3.,
 H 2HTI, 47.900 , 4., 2HV , 50.942 , 5., 2HGR, 51.996 , 3.,
 I 2HMN, 54.9380 , 2., 2HFE, 55.847 , 3., 2HCO, 58.9332 , 2.,
 J 2HNI, 58.710 , 2., 2HCU, 63.540 , 2., 2HZN, 65.370 , 2.,
 K 2HGA, 69.720 , 3., 2HGE, 72.590 , 4., 2HAS, 74.9216 , 3.,
 L 2HSE, 78.960 , 4., 2HBR, 79.909 , -1., 2HKR, 83.800 , 0.,
 M 2HRB, 85.47 , 1., 2HSR, 87.620 , 2., 2HY , 88.905 , 3.,
 N 2HZR, 91.220 , 4., 2HNB, 92.906 , 5., 2HMO, 95.94 , 6.,
 O 2HTC, 99.000 , 7., 2HRU,101.070 , 3., 2HRH,102.905 , 3.,
 P 2HPD,106.400 , 2., 2HAG,107.870 , 1., 2HCD,112.400 , 2.,
 Q 2HIN,114.820 , 3., 2HSN,118.690 , 4., 2HSB,121.750 , 3. /
 DATA ((ATOM(I,J),I=1,3),J=53,101)/

	2HTE,127.600	, 4.,	2HI ,126.9044	,-1.,	2HXE,131.300	, 0.,
S	2HCS,132.905	, 1.,	2HBA,137.340	, 2.,	2HLA,138.910	, 3.,
T	2HCE,140.120	, 3.,	2HPR,140.907	, 3.,	2HND,144.240	, 3.,
U	2HPM,145.000	, 3.,	2HSM,150.350	, 3.,	2HEU,151.960	, 3.,
V	2HGD,157.250	, 3.,	2HTB,158.924	, 3.,	2HDY,162.500	, 3.,
W	2HHO,164.930	, 3.,	2HER,167.260	, 3.,	2HTM,168.934	, 3.,
X	2HYB,173.040	, 3.,	2HLU,174.997	, 3.,	2HHF,178.490	, 4.,
Y	2HTA,180.948	, 5.,	2HW ,183.850	, 6.,	2HRE,186.200	, 7.,
Z	2HOS,190.200	, 4.,	2HIR,192.200	, 4.,	2HPT,195.090	, 4.,
A	2HAU,196.967	, 3.,	2HHG,200.590	, 2.,	2HTL,204.370	, 1.,
B	2HPB,207.190	, 2.,	2HBI,208.980	, 3.,	2HPO,210.000	, 2.,
C	2HAT,210.000	, 0.,	2HRN,222.000	, 0.,	2HFR,223.000	, 1.,
D	2HRA,226.000	, 2.,	2HAC,227.000	, 3.,	2HTH,232.038	, 4.,
E	2HPA,231.000	, 5.,	2HU ,238.030	, 6.,	2HNP,237.000	, 5.,
F	2HPU,242.000	, 4.,	2HAM,243.000	, 3.,	2HCM,247.000	, 3.,
G	2HBK,249.000	, 3.,	2HCF,251.000	, 3.,	2HES,254.000	, 0.,
H	2HD ,2.014102,	1./				

C
C
C

INFORMATION USED IN VARIABLE OUTPUT FORMAT

DATA FMT/3H(1H,4H,3A4,4H,A2,,3HF9.,2H0,,3HF9.,2H0,,3HF9.,2H0,,3HF9.
1.,2H0,,3HF9.,2H0,,3HF9.,2H0,,3HF9.,2H0,,3HF9.,2H0,,3HF9.,2H0,,3HF9.
2.,2H0,,3HF9.,2H0,,3HF9.,2H0,,3HF9.,1H0,1H)/, FB,F0,F1,F2,F3,F4,F5/
31H ,2H0,,2H1,,2H2,,2H3,,2H4,,2H5,/,FMT13/2H13/,FMT9X/3H9X,/,FMTI9
4/3HI9,/
DATA

FP/4HP, A,4HTM ,2H ,1H /
1,FT/4HT, D,4HEG K,4H ,2H /,FH/4HH, C,4HAL/G,2H ,1H /
2,FS/4HS, C,4HAL/(,4HG)(K,2H) /,FM/4HM, M,4HOL W,2HT ,1H /
3,FV/4H(DLV,4H/DLP,4H)T ,2H /,FD/4H(DLV,4H/DLT,2H)P,1H /
4,FC/4HCP, ,4HCAL/,4H(G)(,2HK)/,FG/4HGAMM,4HA (S,2H) ,1H /
5,FL/4HSON ,4HVEL,,4HM/SE,2HC /

C
C
C

INFORMATION USED IN PERFORMANCE OUTPUT

DATA FR1/4HPC/P/, FC1/2HCF/, FN/4HMACH,4H NUM,4HBER ,1H /
1,FR/4HCSTA,4HR, F,4HT/SE,2HC /,FI/4HISP,,4H LB-,4HSEC/,2HLB/
2,FA/4HIVAC,4H,LB-,4HSEC/,2HLB /,FA1/4HAE/A/,FA2/1HT/
END

C
C
C

SUBROUTINE SEARCH

SEARCH TAPE FOR THERMO DATA AND TRANSPORT CROSS SECTIONS OF SPECIES
TO BE CONSIDERED

C
C
C

THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR
IBM 360 MACHINES ONLY

C
C
C

DOUBLE PRECISION COEF,S,EN,ENLN,H0,DELN

C
C
C

INTEGER SUB,OMIT,END,TOOBIG
INTEGER SPECE

C
C

LOGICAL NEWR,WRT

C
C
C

DIMENSION DATE(2,3),MT(4),B(4),OMIT(3,3),NAM(3),TOOBIG(3,50)
DIMENSION SPECE(2,3),TEMPR(20),TABLS(20,3)

C
C

COMMON SPECE , TEMPR , TABLS
COMMON /SPECES/COEF(2,7,150),S(150),H0(150),DELN(150),DUMMY(150),

```

EN(150,13),ENLN(150),A(10,150),SUB(150,3),IUSE(150),TEMP(50,2)
COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),
1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),
2 HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),
3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),
4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)
COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,
1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEWR,NSUB,NSUP,RKT,DETN,SHOCK,
2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,IT,CALCH,NLS,LOGV,
3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQ,PCPLT
COMMON/FLG/JPH1,HTEST,WRT,JQ

```

C
C
C
C
C
C

EQUIVALENCE (DATE,EN),(OMIT,ENLN),(ENDD,END),(TOOBIG,ENLN)

DATA GAS/1HG/,END/3HEND/,ND/4HLAST/

SEARCH FOR THERMO DATA

```

I2B = 0
NC= 0
IX= 0

```

C
C
C

CHECK DIMENSION FOR NUMBER OF SPECIES, CLEAR A(I,J)

```

SUB(1,1) = END
DO 3 I=1,150
IF(A(1,I).EQ.ENDD) GOTO 4
DO 3 J=1,NLM
A(J,I) = 0.
3 CONTINUE
4 MAXNS = I-1

```

C
C
C

READ TEMPERATURE RANGES FOR COEFFICIENTS OF GASEOUS SPECIES.

```

READ(4,5) TLOW,TMID,THIGH
5 FORMAT (3F10.3)
NS = 1

```

C
C
C

BEGIN LOOP FOR READING SPECIES DATA FROM TAPE.

```

7 READ (4,10) (NAM(I),I=1,3),DATE(1,NS),DATE(2,NS),(MT(J),B(J)),
1 J=1,4),PHAZ,T1,T2
10 FORMAT(3A4,6X,2A3,4(A2,F3.0),A1,2F10.3)
IF(NAM(1).EQ.END) GOTO 171
READ (4,20) ((COEF(I,J,NS),J=1,7),I=1,2)
20 FORMAT (5E15.8)
IF(NOMIT.EQ.0) GOTO 810
DO 805 I=1,NOMIT
DO 804 J=1,3
IF(OMIT(J,I).NE.NAM(J)) GOTO 805
804 CONTINUE
GOTO 7
805 CONTINUE
810 DO 820 K=1,4
IF(B(K).EQ.0.) GOTO 825
DO 168 I=1,NLM
IF(LLMT(I).EQ.MT(K)) GOTO 820
168 CONTINUE
IF(NS.GT.MAXNS) GOTO 7

```

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```
      DO 819 J=1,NLM
19  A(J,NS) = 0.
      GOTO 7
820 IF(NS.LE.MAXNS) A(I,NS) = B(K)
825 IF(NS.LE.MAXNS) GOTO 828
      I2B = I2B+1
      DO 826 I=1,3
826 TOOBIG(I,I2B) = NAM(I)
      GOTO 7
828 DO 829 I=1,3
829 SUB(NS,I) = NAM(I)
      IUSE(NS) = 0
      IF(PHAZ.EQ.GAS) GOTO 170
C
C  CONDENSED SPECIES
C
      NC= NC+1
      TEMP(NC,1)= T1
      TEMP(NC,2)= T2
      IX= IX+1
      IF(NS.EQ.1.OR.IUSE(NS-1).EQ.0) GOTO 145
      DO 830 I=1,NLM
      IF(A(I,NS).NE.A(I,NS-1)) GOTO 145
830 CONTINUE
      IX= IX-1
145 IUSE(NS)= -IX
170 NS= NS+1
      GOTO 7
C
C  END CARD HAS BEEN READ.
C
171 NS= NS-1
      NEWR= .FALSE.
      IF(.NOT.WRT) GOTO 173
      WRITE(6,172)
172 FORMAT(42HOSPECIES BEING CONSIDERED IN THIS SYSTEM  )
173 CONTINUE
      DO 174 I=1,NS,5
      I5= I+4
      IF(NS.LT.I5) I5=NS
174 IF(.NOT.WRT) GOTO 177
      WRITE (6,176)(DATE(1,J),DATE(2,J),SUB(J,1),SUB(J,2),SUB(J,3),
1 J=I,I5)
176 FORMAT(5(5X,2A3,2X,3A4))
177 CONTINUE
      IF(I2B.GT.0) GOTO 870
      RETURN
870 WRITE(6,871) I2B
871 FORMAT(35H0INSUFFICIENT STORAGE FOR FOLLOWING,I3,8H SPECIES)
      WRITE(6,880)(TOOBIG(1,J),TOOBIG(2,J),TOOBIG(3,J),J=1,I2B)
880 FORMAT(8(3X,3A4))
      RETURN
      END
C
      SUBROUTINE SAVE
C
C  SAVES OR USES COMPOSITIONS FROM PREVIOUS POINT AS INITIAL ESTIMATES
C
C
C  THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR
```

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IBM 360 MACHINES ONLY

DOUBLE PRECISION COEF, S, EN, ENLN, HO, DELN

LOGICAL VOL, CALCH, IONS, SHOCK, WRT

COMMON /SPECES/COEF(2,7,150),S(150),HO(150),DELN(150),DUMMY(150),
1 EN(150,13),ENLN(150),A(10,150),SUB(150,3),IUSE(150),TEMP(50,2)
COMMON /MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),
1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),
2 HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),
3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),
4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)
COMMON /INDX/IDDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,
1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEW,NSUB,NSUP,RKT,DETN,SHOCK,
2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,IT,CALCH,NLS,LOGV,
3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQ,PCPLT
COMMON /SAVED/SLN(100),IQSAVE,ENSAVE,ENLSAV,LSAVE,JSOLS,JLIQS,
1 LLL,LM,MAXNP,STORE(52,16),XS(20),WMOL(20),IND(20),NM,
2 FIRSTP,FIRSTV
COMMON/FLG/JPH1,HTEST,WRT,JQ

DATA IE/IHE/

IF(ISV)100,10,200

NEXT POINT FIRST T IN SCHEDULE, USE PREVIOUS COMPOSITIONS FOR THIS T

10 IQ1 = IQSAVE
JSOL = JSOLS
JLIQ = JLIQS
ENN = ENSAVE
ENNL = ENLSAV
LL1 = NLM
DO 50 J = 1,NS
IF(.NOT.IONS) GOTO 15
IF(LLMT(NLM).EQ.LSAVE) GOTO 15
IF(LLMT(NLM).EQ.IE) GOTO 13
IF(IUSE(J).NE.-10000) GOTO 15
IUSE(J) = 0
LL1 = NLM+1
GOTO 20
13 IF(SLN(J).NE.0..OR.IUSE(J).NE.0) GOTO 15
LL1 = NLM-1
IUSE(J) = -10000
GOTO 50
15 IF (IUSE(J).EQ.0) GOTO 20
EN (J,NPT) = SLN(J)
IF(IUSE(J).GT.0) IUSE(J) = -IUSE(J)
IF (EN(J,NPT).NE.0.)IUSE(J) = -IUSE(J)
GOTO 50
20 EN(J,NPT) = 0.
ENLN(J) = SLN(J)
IF ((ENLN(J)-ENNL + 18.5).LE.0.) GOTO 50
EN(J,NPT) = 2.718281828459**ENLN(J)
50 CONTINUE
NLM = LL1
GOTO 1000

FIRST T--SAVE COMPOSITIONS FOR FUTURE POINTS WITH THIS T

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```
50 ISV = -ISV
   JSOLS = JSOL
   JLIQS = JLIQ
   IQSAVE = IQ1
   ENSAVE = ENN
   ENLSAV = ENNL
   LSAVE = LLMT(NLM)
   DO 150 J = 1,NS
   SLN(J) = ENLN(J)
   IF(IUSE(J).NE.0) SLN(J)=EN(J,ISV)
150 CONTINUE
C
C USE COMPOSITIONS FROM PREVIOUS POINT
C
200 DO 300 J = 1,NS
   EN(J,NPT) = EN(J,ISV)
300 CONTINUE
1000 RETURN
C
C CALCULATE NEW VALUES OF BO AND HSUBO FOR NEW OF RATIO
C
   ENTRY NEWOF
C
   IF(.NOT.WRT) GOTO 731
   WRITE(6,730) OF
730 FORMAT(6H0OF = ,F10.6)
731 CONTINUE
   EQRAT = 0.
   SUM = OF + 1.
   V1 = (OF*VPLS(1)+VPLS(2))/SUM
   V2 = (OF*VMIN(1)+VMIN(2))/SUM
   IF(V2.NE.0.) EQRAT=ABS(V1/V2)
   IF (RH(1) .NE. 0. .AND. RH(2) .NE. 0.) GOTO 744
   RHOP = RH(2)
   IF (RHOP .EQ. 0.) RHOP = RH(1)
   GOTO 745
744 RHOP = (OF+1.)*RH(1)*RH(2)/(RH(1)+OF*RH(2))
745 DO 747 I=1,NLM
   BO(I) = (OF*BOP(I,1)+BOP(I,2))/SUM
747 CONTINUE
   NPT = 1
   IF(.NOT.CALCH) GOTO 750
   CALL HCALC
   IF(TT.EQ.0.) RETURN
   CALCH = .FALSE.
   IF(OF.NE.0.) HPP(1)=SUM*HPP(1)/OF
   HPP(2) = SUM*HPP(2)
   GOTO 760
750 HSUBO= (OF*HPP(1) + HPP(2))/SUM
760 IC = 0
   JSOL = 0
   JLIQ = 0
   IF(.NOT.WRT) GOTO 781
   WRITE (6,770)
770 FORMAT(1H ,25X,14HEFFECTIVE FUEL,10X,17HEFFECTIVE OXIDANT,12X,7HMI
   LXTURE )
   IF(VOL) WRITE(6,772)
   IF(.NOT.VOL) WRITE(6,774)
```

```

FORMAT(16H INTERNAL ENERGY,14X,6HHPP(2),19X,6HHPP(1),19X,5HHSUBO )
74 FORMAT(9H ENTHALPY,21X,6HHPP(2),19X,6HHPP(1),19X,5HHSUBO )
WRITE(6,776) HPP(2),HPP(1),HSUBO
776 FORMAT(19H (KG-MOL)(DEG K)/KG,E21.8,2E25.8 )
WRITE(6,778)
778 FORMAT(12H0KG-ATOMS/KG,17X,8HBOP(I,2),17X,8HBOP(I,1),18X,5HBO(I))
780 FORMAT(8X,A2,5X,3E25.8)
WRITE(6,780) (LLMT(I),BOP(I,2),BOP(I,1),BO(I),I=1,NLM)
781 CONTINUE
RETURN
END

```

C
C
SUBROUTINE OUT1

C
DOUBLE PRECISION G,X
LOGICAL EQL,FROZ,TP,HP,SP,MOLES,VOL,PUNCH,RKT,WRT

C
DIMENSION NV(13),Z(10,3),HEAD(15),YX(5),YN(5),FSB(3),FRHO(3)
DIMENSION DENSTY(13),ENTLPY(13),ENTRPY(13),SPHEAT(13)

C
COMMON /POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),
1 GAMMAS(13),P(26),T(52),V(13),PPP(13),WM(13),SONVEL(13),TTT(13),
2 VLM(13),TOTN(13)
COMMON /SPECES/COEF(2,7,150),S(150),HO(150),DELN(150),DUMMY(150),
1 EN(150,13),ENLN(150),A(10,150),SUB(150,3),IUSE(150),TEMP(50,2)
COMMON /MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),
1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),
2 HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),
3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),
4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)
COMMON /DOUBLE/ G(20,21), X(20)
COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,
1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEW,NSUB,NSUP,RKT,DETN,SHOCK,
2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,IT,CALCH,NLS,LOGV,
3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQ,PCPLT
COMMON /PERF/PCP(22),VMOC(13),SPIM(13),VACI(13),SUBAR(13),
1 SUPAR(13),APP(13),AEAT(13),CSTR,EQL,FROZ,SSO,AREA,AWT,NFZ,
2 APPL,ARATIO,ELN
COMMON /SAVED/SLN(100),IQSAVE,ENSAVE,ENLSAV,LSAVE,JSOLS,JLIQS,
1 LLL,LM,MAXNP,STORE(52,16),XS(20),WMOL(20),IND(20),NM,
2 FIRSTP,FIRSTV
COMMON /OUP/T/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4),
1 FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2,
2 FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0
COMMON /CONTRL/TRNSPT,FROZN,PUNCH,NODATA
COMMON/DNS/rhoce,pce,GAMAce,SVELce,OFRAT,hce,tce,cpce
COMMON/FLG/JPH1,HTEST,WRT,JQ

C
EQUIVALENCE (V,NV),(Z,H0),(IB,FB)

C
C
HEAD=(1H ,2A4,5(A2,F8.5,3X),5X,F7.5,F13.3,4X,A1,F10.2,F9.4)

C
DATA HEAD/4H(1H ,4H,2A4,2H,5,4H(A2,,4HF8.5 ,4H,3X),2H,5 ,2HX,
1 ,4HF7.5 ,4H,F13 ,4H.3,4 ,4HX,A1 ,4H,F10 ,4H.2,F ,4H9.4)/
DATA FUEL/4HFUEL/,OXID/4HOXID/,ANT/3HANT/,OX/1HO/,IZ/2H00/,
1 YN/2H,1, 2H,2, 2H,3, 2H,4, 2H,5 /,F75/4HF7.5/,
2 YX/3H,57,3H,44,3H,31,3H,18,2H,5 /,F73/4HF7.3/
DATA FRHO/4HRHO,,4H G/C,1HC/

```
IF(.NOT.WRT) GOTO 7
IF(KASE.NE.0) WRITE (6,3) KASE
3 FORMAT (9H CASE NO. ,I8)
IF(.NOT.MOLES) WRITE(6,5)
5 FORMAT (77X,46HWT FRACTION ENERGY STATE TEMP DENSITY/
1 10X,16HCHEMICAL FORMULA,51X,21H(SEE NOTE) CAL/MOL,10X,5HDEG K,
2 4X,4HG/CC )
IF(MOLES) WRITE(6,6)
6 FORMAT (79X,5HMOLES,7X, 33H ENERGY STATE TEMP DENSITY/
1 10X,16HCHEMICAL FORMULA,66X,7HCAL/MOL,10X,13HDEG K G/CC )
7 CONTINUE
DO 15 N=1,NREAC
IF(FOX(N).NE.OX)GOTO 10
HD1 = OXID
HD2 = ANT
GOTO 11
10 HD1 = FUEL
HD2 = FB
11 DO 13 J=1,5
IF(NAME(N,J).EQ.IZ.OR.NAME(N,J).EQ.IB) GOTO 14
13 CONTINUE
J=6
14 J=J-1
HEAD(3)=YN(J)
HEAD(7)=YX(J)
HEAD(9) = F75
IF(PECWT(N).GE.10.) HEAD(9)=F73
IF(.NOT.WRT) GOTO 15
WRITE(6,HEAD) HD1,HD2,(NAME(N,JJ),ANUM(N,JJ),JJ=1,J),PECWT(N),
1 ENTH(N), FAZ(N),RTEMP(N),DENS(N)
15 CONTINUE
FPC = 100./(1.+OF)
IF(.NOT.WRT) GOTO 21
WRITE(6,20) OF,FPC,EQRAT,RHOP
20 FORMAT (1H0,15X, 4H0/F=, F8.4,4X,13HPERCENT FUEL=,F8.4,4X,
1 19HEQUIVALENCE RATIO= ,F7.4,4X,17HREACTANT DENSITY=,F8.4//)
21 CONTINUE
AGV = 9.80665
C
RETURN
C
ENTRY OUT2
FMT(4) = FMT(6)
C
PRESSURE
C
50 IF(R.LT.10.) GOTO 60
CALL EFMT(NPT,FP,PPP)
GOTO 61
60 CALL VARFMT (PPP,NPT)
IF(.NOT.WRT) GOTO 61
WRITE (6,FMT) (FP(I),I=1,4),(PPP(J),J=1,NPT)
61 CONTINUE
Pce=PPP(1)
C
TEMPERATURE
C
64 DO 65 I=1,NPT
NV(I)= TTT(I)+.5
65 CONTINUE
```

```
hce=ttt(1)
FMT(4)= FMT13
FMT(5)= FMTI9
IF(.NOT.WRT) GOTO 62
WRITE (6,FMT) (FT(I),I=1,4),(NV(J),J=1,NPT)
62 CONTINUE
C
C DENSITY
C
DO 70 I=1,NPT
IF(VLM(I).NE.0.) V(I)=1./VLM(I)
DENSTY(I) = V(I)
DNSTY=DENSTY(1)
70 CONTINUE
rhoce=densty(1)
CALL EFMT(NPT,FRHO,V)
C
C ENTHALPY
C
DO 75 I=1,NPT
V(I) = HSUM(I) * R
ENTLPHY(I) = V(I)
75 CONTINUE
hce=entlpy(1)
FMT(5)= FB
IF(R.LT.10.) GOTO 76
CALL EFMT(NPT,FH,V)
FMT(7) = F1
GOTO 77
76 FMT(7) = F1
IF(.NOT.WRT) GOTO 66
WRITE (6,FMT) (FH(I),I=1,4),(V(J),J=1,NPT)
66 CONTINUE
C
C ENTROPY
C
FMT(7)=F4
77 DO 78 I=1,NPT
V(I) = SSUM(I) * R
ENTRPHY(I) = V(I)
78 CONTINUE
IF(.NOT.WRT) GOTO 79
WRITE (6,FMT) (FS(I),I=1,4),(V(J),J=1,NPT)
WRITE (6,80)
80 FORMAT ( 1H )
79 CONTINUE
C
C MOLECULAR WEIGHT
C
FMT(7)= F3
IF(.NOT.WRT) GOTO 81
WRITE (6,FMT) (FM(I),I=1,4),(WM(J),J=1,NPT)
81 CONTINUE
C
C (DLV/DLP)T
C
FMT(7)=F5
IF(.NOT.WRT) GOTO 82
IF(EQL) WRITE(6,FMT) (FV(I),I=1,4),(DLVPT(J),J=1,NPT)
82 CONTINUE
```


(DLV/DLT)P

FMT(7)= F4

IF(.NOT.WRT) GOTO 83

IF(EQL) WRITE(6,FMT) (FD(I),I=1,4),(DLVTP(J),J=1,NPT)

83 CONTINUE

C
C HEAT CAPACITY

IF(R.GT.10.) FMT(7)=F1

DO 85 I=1,NPT

V(I) = CPR(I) * R

SPHEAT(I) = V(I)

85 CONTINUE

cpce=spheat(1)

IF(.NOT.WRT) GOTO 86

WRITE(6,FMT) (FC(I),I=1,4),(V(J),J=1,NPT)

86 CONTINUE

C
C GAMMA(S)

FMT(7) = F4

IF(.NOT.WRT) GOTO 87

WRITE(6,FMT) (FG(I),I=1,4),(GAMMAS(J),J=1,NPT)

87 CONTINUE

GAMAcE=GAMMAS(1)

C
C SONIC VELOCITY

FMT(7)= F1

DO 95 I = 1,NPT

SONVEL(I) = (RR*GAMMAS(I)*TTT(I)/WM(I))**.5

95 CONTINUE

IF(.NOT.WRT) GOTO 96

WRITE(6,FMT) (FL(I),I=1,4),(SONVEL(J),J=1,NPT)

96 CONTINUE

SVELce=SONVEL(1)

C
C PUNCHED CARDS &

IF(.NOT.PUNCH) GOTO 4

DO 1 I=1,NPT

IF(RKT.AND.ISV.EQ.0.AND.MAXNP.GT.0.AND.(I.EQ.1.OR.I.EQ.2)) GOTO 1

PUNCH 2, TTT(I),PPP(I),DENSTY(I),ENTLPY(I),ENTRPY(I),WM(I),

1 DLVPT(I),DLVTP(I),V(I),GAMMAS(I),SONVEL(I),FPC

2 FORMAT (F8.2,2(1X,E12.5),F11.2,F11.4,F11.5/2F11.6,F11.5,F11.6,

1 F10.2,2X,F8.4)

1 CONTINUE

C
C 4 RETURN

C
C ENTRY OUT3

C
C TRA = 5.E-6

IF(TRACE.NE.0.) TRA= TRACE

IF(.NOT.EQL) GOTO 331

C
C MOLE FRACTIONS - EQUILIBRIUM

```

      IF(.NOT.WRT) GOTO 309
      WRITE (6,80)
309  CONTINUE
      FMT(7)= F5
      IF(.NOT.WRT) GOTO 311
      WRITE(6,310)
310  FORMAT(15HOMOLE FRACTIONS //)
311  CONTINUE
      DO 330 K=1,NS
      DO 315 I=1,NPT
      V(I) = EN(K,I)/TOTN(I)
315  CONTINUE
      DO 316 I=1,NPT
      IF(TRACE.EQ.0.) GOTO 317
      IF(V(I).GE.TRACE) GOTO 325
317  IF(V(I).GE.(5.E-6)) GOTO 320
316  CONTINUE
      GOTO 330
320  IF(.NOT.WRT) GOTO 321
      WRITE (6,FMT) SUB(K,1),SUB(K,2),SUB(K,3),FB,(V(I),I=1,NPT)
321  CONTINUE
      GOTO 330
325  FSB(1) = SUB(K,1)
      FSB(2) = SUB(K,2)
      FSB(3) = SUB(K,3)
      CALL EFMT(NPT,FSB,V)
330  CONTINUE
331  IF(.NOT.WRT) GOTO 336
      WRITE(6,335) TRA
335  FORMAT(83H0ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOL
      1E FRACTIONS WERE LESS THAN ,E12.5,28H FOR ALL ASSIGNED CONDITIONS/
      2/)
336  CONTINUE
      LINE= 0
      NN = 1
      IF(EQL) NN=NPT
      DO 350 K=1,NS
      DO 340 I=1,NN
      IF ((EN(K,I)/TOTN(I)).GE.TRA) GOTO 343
340  CONTINUE
      LINE= LINE+1
      Z(LINE,1)= SUB(K,1)
      Z(LINE,2)= SUB(K,2)
      Z(LINE,3)= SUB(K,3)
343  IF ((LINE.NE.10) .AND. K.NE.NS) GOTO 350
      IF (LINE.EQ.0) GOTO 1000
      IF(.NOT.WRT) GOTO 346
      WRITE(6,345) (Z(LN,1),Z(LN,2),Z(LN,3),LN=1,LINE)
345  FORMAT (10(1X,3A4))
346  CONTINUE
      LINE= 0
350  CONTINUE
      IF(.NOT.WRT) GOTO 1000
      IF(.NOT.MOLES) WRITE(6,360)
360  FORMAT(78HONOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXI
      2DANT IN TOTAL OXIDANTS )
1000 RETURN
      END

```

C

SUBROUTINE VARFMT(V,NPT)

DIMENSION V(13)

COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4),
1 FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2,
2 FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0

DO 45 I=1,NPT
K= 2*I+3
FMT(K) = F4
IF (V(I).GE.10.) FMT(K) = F3
IF (V(I).GE.100.) FMT(K) = F2
IF (V(I).GE.10000.) FMT(K) = F1
IF (V(I).GE.1000000.) FMT(K) = F0

45 CONTINUE
RETURN
END

SUBROUTINE EFMT(NPT,AA,V)

LOGICAL WRT

DIMENSION AA(3), V(13), W(13), NE(13), FRMT(7)

COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4),
1 FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2,
2 FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0
COMMON/FLG/JPH1,HTEST,WRT,JQ

DATA FRMT/3H(1H,4H,3A4,4H,11X,4H,13(,4HF7.4,4H,I2),1H)/,F63/4HF6.3
1/,FI3/4H,I3)/,F74/4HF7.4/,FI2/4H,I2)/,F11X/4H,11X/,F2X/3H,2X/

FRMT(5) = F74
FRMT(6) = FI2
J1 = 1
FRMT(3) = F2X
IF(FMT(4).NE.FMT9X) GOTO 130
J1 = 2
FRMT(3) = F11X

130 DO 145 I=J1,NPT
IF(V(I).NE.0.) GOTO 140
W(I) = 0.
NE(I) = 0.
GOTO 145

140 EE = ALOG10(ABS(V(I)))
NE(I) = EE
FE = NE(I)
IF(EE.LE.0..AND.FE.NE.EE) NE(I)=NE(I)-1
IF(IABS(NE(I)).LT.10) GOTO 144
FRMT(5) = F63
FRMT(6) = FI3

144 W(I) = V(I)/10.**NE(I)

145 CONTINUE
IF(.NOT.WRT) GOTO 1000
WRITE(6,FRMT) (AA(I),I=1,3),(W(J), NE(J),J=J1,NPT)
1000 RETURN
END

SUBROUTINE CPHS

...CALCULATES THERMODYNAMIC PROPERTIES FOR INDIVIDUAL SPECIES

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```
COMMON /SPECES/COEF(2,7,150),S(150),HO(150),DELN(150),DUMMY(150),
1 EN(150,13),ENLN(150),A(10,150),SUB(150,3),IUSE(150),TEMP(50,2)
COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),
1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),
2 HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),
3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),
4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)
COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,
1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEWR,NSUB,NSUP,RKT,DETN,SHOCK,
2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,IT,CALCH,NLS,LOGV,
3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQL,PCPLT
```

C

EQUIVALENCE (J,JS1)

C

```
K = 1
IF(TT.LE.TMID) K = 2
KK = 0
CPSUM=0.
90 IF(COEF(K,1,J).NE.0.)GOTO 97
IF (IUSE(J).LT.0) GOTO 100
```

C

C IF COEFFICIENTS ARE ZERO, USE OTHER TEMPERATURE INTERVAL

C

```
KK = K
K = 1
IF (KK.EQ.1) K = 2
97 S(J) = (((COEF(K,5,J)/4.)*TT+ COEF(K,4,J)/3.)*TT+ COEF(K,3,J)/
1 2.)* TT+COEF(K,2,J))*TT+ COEF(K,1,J)*TLN + COEF(K,7,J)
HO(J) = (((COEF(K,5,J)/5.)*TT+ COEF(K,4,J)/4.)*TT+ COEF(K,3,J)/
1 3.)*TT+ COEF(K,2,J)/2.)*TT+ COEF(K,1,J) + COEF(K,6,J)/TT
CPSUM= CPSUM+(((COEF(K,5,J)*TT+ COEF(K,4,J))*TT+ COEF(K,3,J))*TT
1 + COEF(K,2,J))*TT+ COEF(K,1,J))*EN(J,NPT)
IF (KK.EQ.0) GOTO 100
K = KK
KK = 0
100 IF(J.EQ.NS) GOTO 200
J=J+1
GOTO 90
200 RETURN
END
```

C

SUBROUTINE MATRIX

C

C

```
DOUBLE PRECISION G,X
LOGICAL HP,SP,TP,IDEBUG,CONVG,NEWR,VOL,UV,SV,TV,LOGV
```

C

```
COMMON /POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),
1 GAMMAS(13),P(26),T(52),V(13),PPP(13),WM(13),SONVEL(13),TTT(13),
2 VLM(13),TOTN(13)
COMMON /SPECES/COEF(2,7,150),S(150),HO(150),DELN(150),DUMMY(150),
1 EN(150,13),ENLN(150),A(10,150),SUB(150,3),IUSE(150),TEMP(50,2)
COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),
1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),
2 HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),
3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),
4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)
COMMON /DOUBLE/ G(20,21), X(20)
```


CONDENSED SPECIES

```

C
70 KK = KK + 1
   DO 75 I = 1,L
     G(I,KK) = A(I,J)
     G(I,KMAT) = G(I,KMAT) - A(I,J)*EN(J,NPT)
75 CONTINUE
   G(KK,IQ2) = H0(J)
   G(KK,KMAT) = H0(J) - S(J)
   HSUM(NPT) = HSUM(NPT)+ H
   IF(.NOT.SP) GOTO 65
   SSS = SSS + S(J)*EN(J,NPT)
   G(IQ2,KK) = S(J)
65 CONTINUE
   SSS = SSS + G(IQ2,IQ1)
   HSUM(NPT) = HSUM(NPT) + G(IQ1,IQ2)
   G(IQ1,IQ1) = SUMN - ENN

C
C REFLECT SYMMETRIC PORTIONS OF THE MATRIX
C
   ISYM = IQ1
   IF(HP.OR.CONV)ISYM=IQ2
   DO 102 I=1,ISYM
     DO 102 J=I,ISYM
       G(J,I)=G(I,J)
102 CONTINUE

C
C COMPLETE THE RIGHT HAND SIDE
C
   IF(.NOT.CONV) GOTO 140
   IF(.NOT.LOGV) GOTO 175

C
C LOGV = .TRUE.-- SET UP MATRIX TO SOLVE FOR DLVPT
C
   G(IQ1,IQ2) = ENN
   IQ = IQ1 - 1
   DO 135 I = 1,IQ
     G(I,IQ2) = G(I,IQ1)
135 CONTINUE
   GOTO 175
140 DO 145 I=1,L
     X(1)=B0(I)-G(I,IQ1)
     G(I,KMAT) = G(I,KMAT)+X(1)
145 CONTINUE
   G(IQ1,KMAT) = G(IQ1,KMAT)+ENN-SUMN

C
C COMPLETE ENERGY ROW AND TEMPERATURE COLUMN
C
   IF (KMAT .EQ. IQ2) GOTO 185
   IF (SP)ENERGY = S0+ENN-SUMN - SSS
   IF(HP)ENERGY=HSUB0/TT - HSUM(NPT)
   G(IQ2,IQ3)=G(IQ2,IQ3)+ ENERGY
175 G(IQ2,IQ2)= G(IQ2,IQ2)+CPSUM
185 IF(.NOT.VOL.OR.CONV) GOTO 1000

C
C CONSTANT VOLUME MATRIX
C
   IQ =IQ1-1

```

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```
(KMAT.EQ.IQ2) GOTO 230
DO 220 I=1,IQ
G(IQ1,I) = G(IQ2,I)-G(IQ1,I)
G(I,IQ1) = G(I,IQ2)-G(I,IQ1)
G(I,IQ2) = G(I,IQ3)
220 CONTINUE
G(IQ1,IQ1) = G(IQ2,IQ2)-G(IQ1,IQ2)-G(IQ2,IQ1)
G(IQ1,IQ2) = G(IQ2,IQ3)-G(IQ1,IQ3)
IF (UV) G(IQ1,IQ2) = G(IQ1,IQ2) + ENN
GOTO 260
230 DO 240 I=1,IQ
G(I,IQ1) = G(I,IQ2)
240 CONTINUE
260 KMAT = IMAT
IMAT = IMAT-1
1000 RETURN
END

C
SUBROUTINE THERMP

C
LOGICAL HP,SP,TP,UV,SV,NEW, IONS,MOLES,RKT,VOL,TV,
1 CALCH,WRT

C
DIMENSION VL(26)

C
COMMON /POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),
1 GAMMAS(13),P(26),T(52),V(13),PPP(13),WM(13),SONVEL(13),TTT(13),
2 VLM(13),TOTN(13)
COMMON /SPECES/COEF(2,7,150),S(150),HO(150),DELN(150),DUMMY(150),
1 EN(150,13),ENLN(150),A(10,150),SUB(150,3),IUSE(150),TEMP(50,2)
COMMON /MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),
1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AM(2),
2 HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),
3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),
4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)
COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,
1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEW,NSUB,NSUP,RKT,DET,SHOCK,
2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,IT,CALCH,NLS,LOGV,
3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQ,PCPLT
COMMON /OUP/T/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4),
1 FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2,
2 FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0
COMMON/TESTS/ATEST,BTEST,CTEST,DTEST,RTEST,STEST,TTEST,UTEST,VTEST
1,XTEST,YTEST
COMMON/DNS/rhoce,pce,GAMAce,SVELce,OFRAT,hce,tce,cpce
COMMON/FLG/JPH1,HTEST,WRT,JQ

C
EQUIVALENCE (K,ISV),(VL,P),(UV,HP),(TP,TV),(SP,SV)

C
DATA FUJ/4HU,C/

C
IF(T(1).EQ.0.) T(1) = 3800.

C
IOF = 0
95 IOF = IOF+1
OF = OXF(IOF)
CALL NEWOF
IF(TT.EQ.0..AND.CALCH) RTEST = 1.
IF(TT.EQ.0..AND.CALCH) RETURN

C
```

IF ASSIGNED P OR VOLUME

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```
IP = 0
903 IP = IP + 1
PP = P(IP)
VLM(NPT) = VL(IP)

C
C SET ASSIGNED T
C

IT = 0
902 IT = IT + 1
TT = T(IT)
CALL EQLBRM
IF(TT.NE.0.) GOTO 800
IF(NPT.EQ.0) GOTO 1000
800 K = 0
IF(IP.EQ.NP.AND.IT.EQ.NT.OR.TT.EQ.0.) GOTO 860
K = NPT
IF(NPT.NE.13) GOTO 870
860 IF(.NOT.HP.AND.WRT) WRITE(6,5)
5 FORMAT(1H1,41X,48HTHERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED
1)
IF(.NOT.WRT) GOTO 7
IF(HP) WRITE(6,6)
6 FORMAT(1H1,36X,59HTHERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES
LAT ASSIGNED )
7 CONTINUE
IF(.NOT.VOL) GOTO 861
IF(.NOT.WRT) GOTO 13
IF(UV) WRITE(6,10)
10 FORMAT(1H0,62X,7H VOLUME /)
IF(TV) WRITE(6,11)
11 FORMAT(1H0,54X,22HTEMPERATURE AND VOLUME/)
IF(SV) WRITE(6,12)
12 FORMAT(1H0,56X,18HENTROPY AND VOLUME/)
13 CONTINUE
GOTO 862
861 IF(.NOT.WRT) GOTO 862
IF(HP) WRITE(6,20)
20 FORMAT(1H0,62X,10H PRESSURES /)
IF(TP) WRITE(6,21)
21 FORMAT(1H0,53X,24HTEMPERATURE AND PRESSURE/)
IF(SP) WRITE(6,22)
22 FORMAT(1H0,55X,20HENTROPY AND PRESSURE/)
862 CALL OUT1
IF(.NOT.WRT) GOTO 1863
WRITE (6,863)
863 FORMAT (25HOTHERMODYNAMIC PROPERTIES//)
1863 CONTINUE
IF(.NOT.VOL) GOTO 864
FMT(4) = FMT(6)
IF(.NOT.UV) GOTO 864
DO 63 I=1,NPT
FMT(2*I+3) = F2
V(I) = HSUBO*R
63 CONTINUE
IF(.NOT.WRT) GOTO 864
WRITE(6,FMT) FUU, FH(2), FB, FB, (V(I), I=1, NPT)
864 CALL OUT2
CALL OUT3
```


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DTEST = 1.
RETURN

C
C
ENTRY THERM1

DTEST = 0.
RTEST = 0.
VTEST = 0.

865 IF(K.EQ.0 .AND. IOF.EQ.NO) GOTO 1000
IF(IDEBUG.GT.13) IDEBUG=IDEBUG-13
IF(.NOT.WRT) GOTO 1868
WRITE(6,868)

868 FORMAT(1H1)

1868 CONTINUE

IF(NT.EQ.1.AND.NP.EQ.1) GOTO 95
NPT = 0

870 NPT = NPT + 1

IF(.NOT.TP.AND.TT.NE.0.) T(1)=TT
IF(IP.EQ.1.AND.IT.EQ.1) ISV=-ISV
IF(NT.EQ.1) GOTO 871
IF(IT.EQ.NT.OR.TT.EQ.0.) ISV=0

871 CALL SAVE

IF(IT.LT.NT) GOTO 902

IF(IP.LT.NP) GOTO 903

GOTO 95

1000 VTEST = 1.

RETURN

END

APPENDIX D

INFORMATION ON THE COMPUTER PROGRAM

Input

The program requires five input files. Four of these are used by the chemical equilibrium calculation routines. NMLST.DAT replaces the namelist input of the NASA/Lewis code. EVAL.HIN and EVAL.FIN contain the reactant information for hydrogen and the fuel system being tested, and have the same format as specified by the NASA/Lewis code. THERMO.DAT contain the thermodynamic information for the species to be considered. EVAL.GIN is a 10 line file containing the information required by the evaluation program. Contents of each line with the format in parentheses are as follows:

1. Run number, first A-B phase fuel, second (hypersonic) phase fuel, rocket fuel, and the baseline fuel on which all the comparisons are based (A4,4A10).
2. Fuel system identifier. Takes the value of 1 if the same fuel is used to produce the rocket fuel and the hydrogen for both A-B phases; 2 if fuel for the first A-B phase supplies the hydrogen for the second A-B phase and the rocket fuel; 3 if a different fuel is used for each phase; 4 if baseline fuel is used for the first A-B phase and partially for the second phase while the rest of the hydrogen requirement is met by the hydrogen produced during the generation of the rocket phase fuel. Since it was found that all the systems under consideration produced a large excess of rocket fuel, the options 1 and 2 were not used after the first few runs. NOPRT is set to be true if all the printout from the chemical equilibrium calculations are to be suppressed. Otherwise it prints the output for the last set of equilibrium calculations. WRT is set to be false for all cases because otherwise outputs of all the chemical equilibrium calculations will be printed. In this case the output file will have a size of several megabytes. For this reason WRT should be set true only for diagnostic purposes (I2,2L7).

3. Gross lift-off mass in kilograms, subsystem mass for hydrogen vehicle in kilograms, subsystem mass for the test vehicle in kilograms, density of the baseline fuel in kg/m^3 , and the rocket phase propulsion efficiency (5E12.6).
4. Hypersonic phase switchover Mach number, Mach number at which the first intermediate dynamic pressure and angle of attack values are given, Mach number at which the second intermediate dynamic pressure and angle of attack values are given, switchover Mach number to rocket propulsion (4F8.3).
5. Dynamic pressure at the start of hypersonic phase in Pa, dynamic pressure at first intermediate point in Pa, dynamic pressure at the second intermediate point in Pa, dynamic pressure at the switchover point to rocket propulsion (4F8.3).
6. Angle of attack at the start of hypersonic phase in degrees, angle of attack at the first intermediate point in degrees, and the angle of attack at the second intermediate point in degrees (3f8.3)
7. Average thrust to drag ratio for the first air-breathing propulsion phase, thrust to drag ratio with the test fuel at the beginning of the second (hypersonic) air-breathing propulsion phase, thrust to drag ratio with the baseline fuel at the second air-breathing propulsion phase, and the step size (altitude increment) in meters for the integral in the mass ratio correlation for the hypersonic flight phase (3F10.6,E12.6).
8. Heat of combustion per unit mass for the baseline fuel in J/kg, heat of combustion of the fuel for the first air-breathing phase in J/kg, heat of combustion of the additional rocket fuel in J/kg, heat of combustion of the fuel for the second (hypersonic) air-breathing phase in J/kg, heat of combustion of the rocket fuel produced during

the air-breathing propulsion phase in J/kg, and the propulsion efficiency during air-breathing propulsion (6E12.6).

9. Fuel to oxygen mass ratio for rocket fuel produced during air-breathing phase, fuel to oxygen mass ratio for the additional rocket fuel, ratio of the mass of rocket fuel produced during air-breathing propulsion per unit mass of hydrogen produced, ratio of the mass of additional equipment and supplies required for the generation of hydrogen and rocket fuel to the mass of hydrogen produced (4E12.6).
10. Tankage mass per unit propellant volume in kg/m^3 for the additional rocket fuel, tankage mass per unit propellant volume in kg/m^3 for the first air-breathing phase fuel, tankage mass per unit volume in kg/m^3 for the second air-breathing phase (when FTEST is 4 this is for the substance producing the rocket fuel and supplementary hydrogen), density of second air-breathing phase fuel (or the density of the substance producing the rocket fuel and the supplementary hydrogen when FTEST is 4) in kg/m^3 , density of the first air-breathing phase fuel in kg/m^3 , and the density of the additional rocket fuel in kg/m^3 (6F10.6).

Namelist Input (NMLST.DAT)

Because the available fortran compiler did not accommodate namelist input, the data file NMLST.DAT is used for this purpose. It is a one line data file containing the following information: KASE, P(1), MIX(1), HP, NSQM, FA, ERATIO, IONS, SIUNIT (I3,E12.6,F10.6,6L7).

The value specified here for P(1) does not have any significance because the program uses the combustion chamber inlet pressure PCI for P(1), but kept here for cases in which chemical equilibrium at another pressure may be required. For assigned T and P cases T is equated to the combustion chamber inlet temperature TCI by the program and there is no need to specify a temperature in the namelist

input. HP is set to .TRUE. For constant pressure combustion calculations. For assigned T and P calculations the program changes HP to .FALSE. and makes TP .TRUE. The mixture composition can be specified as an equivalence ratio or fuel to air mass ratio by setting either the ERATIO or FA true. SIUNIT should be specified as true because the other sections of the program uses SI units.

APPENDIX E

RUN NUMBER =003A

BASELINE FUEL = LH2

PHASE 1FUEL = SH2

PHASE 2FUEL = SH2

PHASE 3FUEL = SH2

LIFT-OFF MASS = 300000. KG

ORBITAL ALTITUDE = 200.000 KM

ORBITAL VELOCITY = 8030.00 M/S

** VEHICLE PARAMETERS **

	BASE VEHICLE RUNNING ON H2	VEHICLE RUNNING ON TEST FUEL(S)

A-B phase fuel volume (m3)	829.063	706.730
Rocket phase propellant volume (m3)	222.679	203.225
Total vehicle volume (m3)	1617.26	1432.94
Characteristic dimension (m)	31.8618	30.6022
Mass of vehicle at orbit (kg)	148310.	148837.
Mass of vehicle at switchover (kg)	241966.	242826.
A-B phase fuel mass (kg)	58034.4	57174.5
Rocket propellant mass (kg)	93655.9	93988.8
Rocket fuel produced (kg)	.000000	.000000
Additional rocket fuel (kg)	.000000	.000000
Excess rocket fuel (kg)	.000000	.000000
Total propellant mass consumed (kg)	151690.	151163.
Thrust structure mass (kg)	2647.80	2647.80
Propellant tankage mass (kg)	11659.0	8305.69
Fuel Production system mass (kg)	.000000	.000000
Thermal protection mass (kg)	32197.6	30781.6
Engine mass (kg)	18000.0	18000.0
Subsystem mass (kg)	10000.0	10000.0
Payload mass (kg)	73805.2	79101.7
Rocket specific impulse (s)	901.733	901.733
Capture area (m2)	33.4702	33.0585

** FLIGHT PROFILE **

	PHASE1 AB	CHANGE TO HYPERSONIC	PHASE2 AB	CHANGE TO ROCKET
Z (M)		17936.6	26996.2	32312.9
MA		3.00000	6.00000	9.00000
Q (PA)	47882.0	47882.0	47882.0	47882.0
TETA (DEG)		2.00000	2.00000	2.00000

** HYPERSONIC PHASE PROFILE **

ALTITUDE (M)	MACH NUMBER	SPECIFIC IMPULSE, H2 (S)	SPECIFIC IMPULSE, FUEL (S)	EFF. FUEL SPEC. IMPULS H2, (S)	EFF. FUEL SPEC. IMPULS FUEL, (S)
17936.6	2.99790	1762.46	1762.46	1337.77	1337.77
19736.6	3.44055	1935.25	1935.25	1495.10	1512.37
21536.6	3.94856	2018.67	2018.67	1560.84	1578.79
23336.6	4.53159	2042.89	2042.89	1564.80	1583.55
25136.6	5.20069	2053.10	2053.10	1551.82	1571.49
26936.6	5.96860	2029.95	2029.95	1502.10	1522.80
28736.6	6.84988	1998.77	1998.77	1440.45	1462.35
30536.6	7.86130	1960.08	1960.08	1366.82	1390.09
32336.6	9.02205	1905.07	1905.07	1271.72	1296.56
36236.6	12.0455	1757.26	1757.26	1012.47	1041.68

ALTITUDE (M)	MACH NUMBER	THRUST/DRAG RATIO, H2	THRUST/DRAG RATIO, FUEL	DRAG H2, (N)	DRAG FUEL, (N)	THRUST H2, (N)	THRUST FUEL, (N)	AIR FLOW H2, (KG/S)	AIR FLOW FUEL, (KG/S)
17936.6	2.99790	4.15000	4.15000	429489.	424207.	.178238E+07	.176046E+07	3581.03	3536.99
19736.6	3.44055	4.39681	4.57630	387144.	367386.	.170220E+07	.168127E+07	3114.58	3076.27
21536.6	3.94856	4.40915	4.58914	350248.	332372.	.154430E+07	.152530E+07	2708.88	2675.57
23336.6	4.53159	4.27305	4.44749	318099.	301864.	.135925E+07	.134253E+07	2356.04	2327.06
25136.6	5.20069	4.09573	4.26293	290086.	275280.	.118811E+07	.117350E+07	2049.15	2023.95
26936.6	5.96860	3.84566	4.00265	265677.	252117.	.102170E+07	.100914E+07	1782.23	1760.32
28736.6	6.84988	3.57996	3.72610	244408.	231934.	874971.	864210.	1550.09	1531.02
30536.6	7.86130	3.30389	3.43876	225876.	214348.	746269.	737091.	1348.18	1331.60
32336.6	9.02205	3.00793	3.13072	209728.	199024.	630846.	623088.	1172.57	1158.15
36236.6	12.0455	2.35938	2.45570	182277.	172974.	430062.	424773.	866.603	855.945

RUN NUMBER =0032

PHASE 1 FUEL = CH4-H2 GEL
PHASE 2 FUEL = CH4-H2 GEL
PHASE 3 FUEL = CH4-H2 GEL

LIFT-OFF MASS = 300000. KG
ORBITAL ALTITUDE = 200.000 KM
ORBITAL VELOCITY = 8030.00 M/S

** VEHICLE PARAMETERS **

	BASE VEHICLE RUNNING ON LH2	VEHICLE RUNNING ON TEST FUEL(S)

A-B phase fuel volume (m3)	976.894	822.239
Rocket phase propellant volume (m3)	275.678	254.024
Total vehicle volume (m3)	1878.34	1649.14
Characteristic dimension (m)	33.4915	32.0698
Mass of vehicle at orbit (kg)	115671.	110390.
Mass of vehicle at switchover (kg)	231617.	229542.
A-B phase fuel mass (kg)	68382.6	70457.7
Rocket propellant mass (kg)	115946.	119153.
Rocket fuel produced (kg)	.000000	.000000
Additional rocket fuel (kg)	.000000	.000000
Excess rocket fuel (kg)	.000000	.000000
Total propellant mass consumed (kg)	184329.	189610.
Thrust structure mass (kg)	2647.80	2647.80
Propellant tankage mass (kg)	13978.6	9818.49
Fuel Production system mass (kg)	.000000	.000000
Thermal protection mass (kg)	29005.2	26775.7
Engine mass (kg)	18000.0	18000.0
Payload mass (kg)	42039.4	43147.8
Rocket specific impulse (s)	576.996	547.256
Inlet area (m2)	35.2658	34.9497

** FLIGHT PROFILE **

PHASE1 AB

CHANGE TO
HYPERSONIC

PHASE2 AB

CHANGE TO
ROCKET

Z (M)		17936.6	26996.2	32312.9	36190.4
MA		3.00000	6.00000	9.00000	12.00000
Q (PA)	47882.0	47882.0	47882.0	47882.0	
TETA (DEG)		2.00000	2.00000	2.00000	

** HYPERSONIC PHASE PROFILE **

ALTITUDE (M)	MACH NUMBER	SPECIFIC IMPULSE, LH2 (S)	SPECIFIC IMPULSE, FUEL (S)	EFF. FUEL SPEC. IMPULS LH2, (S)	EFF. FUEL SPEC. IMPULS FUEL, (S)
17936.6	2.99790	1762.46	1679.95	1243.87	1184.49
19736.6	3.44055	1935.25	1843.84	1387.77	1338.98
21536.6	3.94856	2018.67	1922.29	1438.89	1387.26
23336.6	4.53159	2042.89	1944.75	1426.41	1375.46
25136.6	5.20069	2053.10	1952.77	1395.11	1344.75
26936.6	5.96860	2029.95	1930.44	1325.13	1278.79
28736.6	6.84988	1998.77	1899.46	1239.11	1196.63
30536.6	7.86130	1960.08	1861.19	1141.02	1103.15
32336.6	9.02205	1905.07	1814.46	1020.23	995.412
36236.6	12.0455	1757.26	1660.76	704.681	686.920

ALTITUDE (M)	MACH NUMBER	THRUST/DRAG RATIO, LH2	THRUST/DRAG RATIO, FUEL	DRAG LH2, (N)	DRAG FUEL, (N)	THRUST LH2, (N)	THRUST FUEL, (N)	AIR FLOW LH2, (KG/S)	AIR FLOW FUEL, (KG/S)
17936.6	2.99790	4.15000	4.15000	452530.	446350.	.187800E+07	.185235E+07	3773.14	3739.33
19736.6	3.44055	4.39681	4.59525	407914.	384797.	.179352E+07	.176824E+07	3281.67	3252.26
21536.6	3.94856	4.40915	4.60568	369038.	348124.	.162714E+07	.160335E+07	2854.21	2828.63
23336.6	4.53159	4.27305	4.46215	335164.	316170.	.143217E+07	.141080E+07	2482.43	2460.19
25136.6	5.20069	4.09573	4.27326	305648.	288327.	.125185E+07	.123209E+07	2159.08	2139.73
26936.6	5.96860	3.84566	4.01169	279930.	264066.	.107651E+07	.105935E+07	1877.85	1861.02
28736.6	6.84988	3.57996	3.73190	257520.	242926.	921911.	906577.	1633.25	1618.61
30536.6	7.86130	3.30389	3.44136	237994.	224506.	786305.	772606.	1420.51	1407.78
32336.6	9.02205	3.00793	3.14261	220979.	208456.	664690.	655096.	1235.48	1224.40
36236.6	12.0455	2.35938	2.44599	192056.	181172.	453134.	443145.	913.094	904.911

RUN NUMBER =012A

BASELINE FUEL = LH2

PHASE 1FUEL = LH2

PHASE 2FUEL = H2(B2H6)

PHASE 3FUEL = B

LIFT-OFF MASS = 300000. KG

ORBITAL ALTITUDE = 200.000 KM

ORBITAL VELOCITY = 8030.00 M/S

** VEHICLE PARAMETERS **

	BASE VEHICLE RUNNING ON H2	VEHICLE RUNNING ON TEST FUEL(S)
	-----	-----
A-B phase fuel volume (m3)	829.063	763.057
Rocket phase propellant volume (m3)	222.679	87.7979
Total vehicle volume (m3)	1617.26	1356.11
Characteristic dimension (m)	31.8618	30.0452
Mass of vehicle at orbit (kg)	148310.	98039.2
Mass of vehicle at switchover (kg)	241966.	243215.
A-B phase fuel mass (kg)	58034.4	56784.9
Rocket propellant mass (kg)	93655.9	145176.
Rocket fuel produced (kg)	.000000	45086.4
Additional rocket fuel (kg)	.000000	.000000
Excess rocket fuel (kg)	.000000	.000000
Total propellant mass consumed (kg)	151690.	201961.
Thrust structure mass (kg)	2647.80	2647.80
Propellant tankage mass (kg)	11659.0	7458.45
Fuel Production system mass (kg)	.000000	12.6109
Thermal protection mass (kg)	32197.6	22958.7
Engine mass (kg)	18000.0	18000.0
Subsystem mass (kg)	10000.0	10000.0
Payload mass (kg)	73805.2	36961.7
Rocket specific impulse (s)	901.733	485.804
Capture area (m2)	33.4702	32.8706

** FLIGHT PROFILE **

	PHASE1 AB	CHANGE TO HYPERSONIC	PHASE2 AB	CHANGE TO ROCKET
Z (M)		17936.6	26996.2	36190.4
MA		3.00000	6.00000	12.00000
Q (PA)	47882.0	47882.0	47882.0	47882.0
TETA (DEG)		2.00000	2.00000	2.00000

** HYPERSONIC PHASE PROFILE **

ALTITUDE (M)	MACH NUMBER	SPECIFIC IMPULSE, H2 (S)	SPECIFIC IMPULSE, FUEL (S)	EFF. FUEL SPEC. IMPULS H2, (S)	EFF. FUEL SPEC. IMPULS FUEL, (S)
17936.6	2.99790	1762.46	1762.46	1337.77	1337.77
19736.6	3.44055	1935.25	1935.25	1495.10	1520.39
21536.6	3.94856	2018.67	2018.67	1560.84	1587.14
23336.6	4.53159	2042.89	2042.89	1564.80	1592.27
25136.6	5.20069	2053.10	2053.10	1551.82	1580.62
26936.6	5.96860	2029.95	2029.95	1502.10	1532.42
28736.6	6.84988	1998.77	1998.77	1440.45	1472.53
30536.6	7.86130	1960.08	1960.08	1366.82	1400.90
32336.6	9.02205	1905.07	1905.07	1271.72	1308.11
36236.6	12.0455	1757.26	1757.26	1012.47	1055.26

ALTITUDE (M)	MACH NUMBER	THRUST/DRAG RATIO, H2	THRUST/DRAG RATIO, FUEL	DRAG H2, (N)	DRAG FUEL, (N)	THRUST H2, (N)	THRUST FUEL, (N)	AIR FLOW H2, (KG/S)	AIR FLOW FUEL, (KG/S)
17936.6	2.99790	4.15000	4.15000	429489.	421795.	.178238E+07	.175045E+07	3581.03	3516.88
19736.6	3.44055	4.39681	4.66483	387144.	358365.	.170220E+07	.167171E+07	3114.58	3058.79
21536.6	3.94856	4.40915	4.67791	350248.	324211.	.154430E+07	.151663E+07	2708.88	2660.36
23336.6	4.53159	4.27305	4.53352	318099.	294452.	.135925E+07	.133490E+07	2356.04	2313.83
25136.6	5.20069	4.09573	4.34539	290086.	268521.	.118811E+07	.116683E+07	2049.15	2012.44
26936.6	5.96860	3.84566	4.08008	265677.	245927.	.102170E+07	.100340E+07	1782.23	1750.31
28736.6	6.84988	3.57996	3.79818	244408.	226239.	874971.	859298.	1550.09	1522.32
30536.6	7.86130	3.30389	3.50528	225876.	209085.	746269.	732901.	1348.18	1324.03
32336.6	9.02205	3.00793	3.19128	209728.	194137.	630846.	619546.	1172.57	1151.57
36236.6	12.0455	2.35938	2.50320	182277.	168727.	430062.	422358.	866.603	851.080

RUN NUMBER =035A

BASELINE FUEL = LH2

PHASE 1FUEL = LH2

PHASE 2FUEL = H2(C6H12)

PHASE 3FUEL = C6H6

LIFT-OFF MASS = 300000. KG

ORBITAL ALTITUDE = 200.000 KM

ORBITAL VELOCITY = 8030.00 M/S

** VEHICLE PARAMETERS **

	BASE VEHICLE RUNNING ON H2	VEHICLE RUNNING ON TEST FUEL(S)
	-----	-----
A-B phase fuel volume (m3)	829.063	830.993
Rocket phase propellant volume (m3)	222.679	113.943
Total vehicle volume (m3)	1617.26	1478.42
Characteristic dimension (m)	31.8618	30.9226
Mass of vehicle at orbit (kg)	148310.	70479.6
Mass of vehicle at switchover (kg)	241966.	242650.
A-B phase fuel mass (kg)	58034.4	57349.9
Rocket propellant mass (kg)	93655.9	172171.
Rocket fuel produced (kg)	.000000	42275.4
Additional rocket fuel (kg)	.000000	.000000
Excess rocket fuel (kg)	.000000	.000000
Total propellant mass consumed (kg)	151690.	229520.
Thrust structure mass (kg)	2647.80	2647.80
Propellant tankage mass (kg)	11659.0	8403.76
Fuel Production system mass (kg)	.000000	32.7336
Thermal protection mass (kg)	32197.6	19169.6
Engine mass (kg)	18000.0	18000.0
Subsystem mass (kg)	10000.0	10000.0
Payload mass (kg)	73805.2	12225.7
Rocket specific impulse (s)	901.733	357.027
Capture area (m2)	33.4702	33.1429

** FLIGHT PROFILE **

	PHASE1 AB	CHANGE TO HYPERSONIC	PHASE2 AB	CHANGE TO ROCKET
Z (M)		17936.6	26996.2	32312.9
MA		3.00000	6.00000	9.00000
Q (PA)	47882.0	47882.0	47882.0	47882.0
TETA (DEG)		2.00000	2.00000	2.00000

** HYPERSONIC PHASE PROFILE **

ALTITUDE (M)	MACH NUMBER	SPECIFIC IMPULSE, H2 (S)	SPECIFIC IMPULSE, FUEL (S)	EFF. FUEL SPEC. IMPULS H2, (S)	EFF. FUEL SPEC. IMPULS FUEL, (S)
17936.6	2.99790	1762.46	1762.46	1337.77	1337.77
19736.6	3.44055	1935.25	1935.25	1495.10	1508.80
21536.6	3.94856	2018.67	2018.67	1560.84	1575.08
23336.6	4.53159	2042.89	2042.89	1564.80	1579.67
25136.6	5.20069	2053.10	2053.10	1551.82	1567.42
26936.6	5.96860	2029.95	2029.95	1502.10	1518.52
28736.6	6.84988	1998.77	1998.77	1440.45	1457.82
30536.6	7.86130	1960.08	1960.08	1366.82	1385.27
32336.6	9.02205	1905.07	1905.07	1271.72	1291.42
36236.6	12.0455	1757.26	1757.26	1012.47	1035.64

ALTITUDE (M)	MACH NUMBER	THRUST/DRAG RATIO, H2	THRUST/DRAG RATIO, FUEL	DRAG H2, (N)	DRAG FUEL, (N)	THRUST H2, (N)	THRUST FUEL, (N)	AIR FLOW H2, (KG/S)	AIR FLOW FUEL, (KG/S)
17936.6	2.99790	4.15000	4.15000	429489.	425289.	.178238E+07	.176495E+07	3581.03	3546.01
19736.6	3.44055	4.39681	4.53798	387144.	371433.	.170220E+07	.168556E+07	3114.58	3084.12
21536.6	3.94856	4.40915	4.55071	350248.	336034.	.154430E+07	.152919E+07	2708.88	2682.39
23336.6	4.53159	4.27305	4.41024	318099.	305189.	.135925E+07	.134596E+07	2356.04	2333.00
25136.6	5.20069	4.09573	4.22723	290086.	278313.	.118811E+07	.117649E+07	2049.15	2029.11
26936.6	5.96860	3.84566	3.96913	265677.	254895.	.102170E+07	.101171E+07	1782.23	1764.80
28736.6	6.84988	3.57996	3.69490	244408.	234489.	874971.	866414.	1550.09	1534.93
30536.6	7.86130	3.30389	3.40997	225876.	216709.	746269.	738971.	1348.18	1334.99
32336.6	9.02205	3.00793	3.10450	209728.	201216.	630846.	624677.	1172.57	1161.10
36236.6	12.0455	2.35938	2.43514	182277.	174880.	430062.	425856.	866.603	858.128