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*III—Hydrogen Gas Fuel  
and Dry Air*

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National Aeronautics  
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**Scientific and Technical  
Information Branch**

## Summary

A series of computations has been made to produce the equilibrium temperature and gas composition for hydrogen gas fuel and dry air. The computed tables and figures provide combustion gas property data for pressures from 0.5 to 50 atmospheres and equivalence ratios from 0 to 2.0. Only sample tables and figures are provided in this report. The complete set of tables and figures is provided on four microfiche films supplied with this report.

## Introduction

A series of computations was made to determine the equilibrium properties of combustion gas products resulting from the combustion of hydrogen gas fuel and dry air. During combustion research it is important that the properties of combustion gases be readily available and in a form that is convenient and useful to the designer and researcher.

In the past, the combustion gas properties of gas turbine fuels as well as a variety of other hydrocarbon fuels have been computed and reported (refs. 1 to 5). These reports have been used extensively at NASA and throughout industry. The computational schemes that have been developed over the years by Huff, Gordon, Zeleznik, and McBride (refs. 6 to 8) form the basis for these reports and have been used to compute combustion gas properties for a wide spectrum of fuel and oxidant combinations. Often, however, the tables and charts have not been prepared for specific fuels. For example, the data of reference 5 are in a tabular form for hydrogen-carbon (H/C) ratios of 1.7, 2.0, and 2.1 for a range of assigned pressures, temperatures, and fuel-air mixtures. The data in this report also include combustion thermodynamic properties for a range of inlet-air temperatures, but the data herein are plotted to facilitate their use. The resulting figures have proven to be extremely useful in combustion research, and copies of such figures have been prepared for a wide variety of fuels. Because of the numerous requests for these figures as well as the interest in high pressure combustion research (ref. 9), we have decided to prepare a new series of figures and tables and extend the applicable range of

the parameters covered. The first two reports of this series listed data from combustion of ASTM Jet A and natural gas with dry air (refs. 10 and 11).

This report presents tables and figures for the combustion gas properties of hydrogen gas fuel and dry air for pressures from 0.5 to 50 atmospheres, inlet-air temperatures from 250 to 1150 K, and equivalence ratios from 0 to 2. Only sample tables and figures are provided in this report. The complete set of tables and figures is provided on the four microfiche films supplied with this report.

## Procedure

The computations for this report were performed using the NASA Lewis chemical equilibrium computer program documented in reference 8 by Gordon and McBride. The computational method uses a free energy minimization method assuming all gases are ideal and interaction among phases can be neglected. The possible products of reaction are Ar, CO, CO<sub>2</sub>, H, HO<sub>2</sub>, H<sub>2</sub>, H<sub>2</sub>O(l), H<sub>2</sub>O, NO, NO<sub>2</sub>, N<sub>2</sub>, O, OH, and O<sub>2</sub>. These data, the atomic weights, and physical constants are the same as those used in reference 5. The lower heat of combustion of hydrogen gas, used in the computations, was obtained from reference 12 ( $11\,988 \times 10^4$  J/kg).

Charts of various useful combustion gas properties were also generated and plotted using computer programs. In the past, these figures had to be generated by crossplotting values from the tables. It was possible to avoid the manual crossplotting of tabular data by having the computer calculate the desired values for a given set of input parameters. For example, the plots in figure 1 are of equilibrium combustion temperature generated over a range of inlet-air temperatures, pressures, and fuel-air ratios. This was done by selecting the final equilibrium combustion temperature, assigning a pressure and fuel-air ratio, and then computing, in an iterative manner, the required value of inlet-air temperature. These computed values were then stored as a data set and figures were produced by the computer. In regions where the results became highly nonlinear, additional computations were performed in order to present the computed results with the same level of accuracy. A careful examination of these regions shows that the curve fit consists of very

short linear segments. In a similar fashion, an appropriate iterative procedure was used to produce the other combustion gas property figures.

## Results

The computation procedure was used to produce the tables and the figures that are presented with this report. The major portion of the information is included on the four microfiche films enclosed at the back of this report. Only sample tables and figures are shown and discussed within the report.

### Tabular Listing

The computations are listed in tabular form on the microfiche. Table I(a) is a copy of a typical listing of the combustion gas properties and species. Included in each table are the following:

(1) The case number and description of reactants, the oxidant-fuel weight ratio (O/F), the fuel-air weight ratio (F/A), the percent fuel, and the equivalence ratio  $\phi$ , which is the ratio of the F/A value to the stoichiometric F/A value, are included. The variation or change in case number has been used to specify a different inlet-air temperature; e.g., case 92 (shown) is 250 K; case 94 is 600 K; case 98 is 1150 K.

(2) Combustion gas properties:

- (a) Equilibrium temperature,  $T$ , K and  $^{\circ}\text{F}$
- (b) Density,  $\rho$ , g/cc
- (c) Molecular weight,  $M$
- (d) Specific heat (at constant pressure),  $C_p$ , cal/g-K
- (e) Isentropic exponent,  $\gamma$  ( $s$ ) (as defined in ref. 8)
- (f) Sonic velocity, m/sec

(3) Mole fractions of the various combustion gas species are given when the concentration is equal to or greater than 5 parts per million by volume (ppm).

The listing at the beginning of table I(a) is the input information on the fuel and oxidant. Listed are, from left to right, the fuel and oxidant atomic formulas, the weight fraction of each component, the heats of formation, and the inlet temperature (fuel was introduced at 298 K and air for case 92 is 250 K). This is a typical input listing used by Gordon in reference 5. Table I(a) lists the gas properties and species concentrations for 1820 different combinations of parametric conditions. The parameters and values used are as follows:

- (1) Combustion pressure, atm: 0.5, 1, 1.5, 2, 3, 4, 6, 10, 15, 20, 30, 40, 50
- (2) Inlet air temperature, K: 250, 400, 600, 800, 1000, 1100, 1150 (case numbers 92 through 98, respectively)

- (3) Equivalence ratio,  $\phi$ : 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.85, 0.9, 0.95, 1.0, 1.05, 1.10, 1.15, 1.2, 1.4, 1.6, 1.8, 2.0

Information contained in table I(a) has been used to generate figures 1, 2, 3, and 6.

Table I(b) lists the combustion gas properties for different combinations of parametric conditions. These tables were computed by assigning pressure, temperature, and fuel-air ratio and then performing iterative calculations to obtain equilibrium composition and properties. The parameters used are the following:

- (1) Pressure, atm: 0.5 to 50 (in steps as indicated previously)
- (2) Temperature, K: 300 to 2800 in 100 K increments
- (3) Fuel-air ratio (weight): 0.000 to 0.100 in increments of 0.010

The case number 0 as listed with the various sections of table I(b) has no significance to any of the data listed in table I(b). Information contained in table I(b) has been used to generate figures 4 and 5.

Additional computations, not listed in table I(a) or I(b), were performed to obtain a more accurate presentation of the nonlinear portions of the curves.

### Graphical Presentations

Some typical figures have been included to illustrate the nature of the figures available on the included microfiche. Table II is a listing of the parameter variations and the range of computed gas properties for each of the six figures presented herein. Figure 1 gives computed values showing the effect of varying the inlet-air temperature, fuel-air ratio, and combustion pressure on equilibrium gas temperature. This figure covers pressures from 4 to 50 atmospheres. Figures at lower pressures, 0.5 to 4 atmospheres, are available on the microfiche.

Figure 2 is similar to figure 1 except that the equilibrium temperature is plotted as a function of fuel-air ratio for various values of inlet-air temperature at a single specified level of combustion pressure; in this case, 1 atmosphere.

Figure 3 is similar to figure 2 except that temperature rise values are plotted versus fuel-air ratio for a range of inlet-air temperatures, again at the 1-atmosphere pressure level. Curves at other pressure levels are to be found on the microfiche.

Figure 4 presents the variation in the isentropic exponent  $\gamma$  (ref. 8) as a function of the mixture temperature for various values of fuel-air ratio at single values of combustion pressure; again, at the 1-atmosphere pressure level. For the purposes of this report, mixture temperature and equilibrium temperature may be used interchangeably.

Figure 5 presents the variation in mixture molecular weight as a function of mixture temperature for various fuel-air ratios at specified levels of combustion pressure.

Figure 6 presents the relationship between the computed equilibrium temperature as a function of the initial temperature for various values of the equivalence ratio ( $\phi$ ) at specified pressure levels.

## Summary of Results

Advanced computational schemes have been used to produce a series of tables and figures specifically for the combustion properties of hydrogen gas fuel and dry air. Complete tabular listings and graphical representations are provided on the four enclosed microfiche.

Lewis Research Center  
National Aeronautics and Space Administration  
Cleveland, Ohio, April 9, 1985

## References

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TABLE I.—CONCLUDED.

(b) Assigned temperature, pressure, and fuel-air ratio

CASE= 0		O/F=100.0000		F/A= 0.01000		PERCENT FUEL= 0.9901		PHI= 0.3430	
P, ATM	0.5000	0.5000	0.5000	0.5000	0.5000	0.5000	0.5000	0.5000	0.5000
P, PSIA	7.3	7.3	7.3	7.3	7.3	7.3	7.3	7.3	7.3
T, DEG K	2800.0	2700.0	2500.0	2400.0	2300.0	2200.0	2100.0	2000.0	1800.0
T, DEG F	4580.3	4400.3	4000.3	3860.3	3680.3	3500.3	3320.3	3140.3	2780.3
RHO, G/CC	5.7401-5	6.0154-5	6.5824-5	6.8825-5	7.1999-5	7.5397-5	7.9071-5	8.3079-5	9.2369-5
M, MOL WT	26.377	26.655	27.006	27.108	27.177	27.222	27.251	27.269	27.286
CP, CAL/(G)(K)	0.9337	0.7886	0.6711	0.5794	0.4583	0.4206	0.3931	0.3731	0.3584
GAMMA(S)	1.1481	1.1565	1.1674	1.1805	1.2096	1.2338	1.2369	1.2484	1.2585
SON VEL,M/SEC	1006.6	986.9	953.2	937.8	922.6	906.8	890.2	872.5	853.7
MOLE FRACTIONS									
AR	0.00841	0.00849	0.00856	0.00861	0.00864	0.00866	0.00868	0.00868	0.00869
CO	0.00011	0.00008	0.00006	0.00004	0.00002	0.00001	0.00001	0.00000	0.00000
CO2	0.00016	0.00019	0.00022	0.00024	0.00026	0.00027	0.00027	0.00028	0.00028
H	0.01127	0.00661	0.00368	0.00194	0.00096	0.00045	0.00019	0.00008	0.00003
H2O	0.00002	0.00002	0.00002	0.00001	0.00001	0.00001	0.00001	0.00000	0.00000
H2	0.00959	0.00685	0.00465	0.00301	0.00185	0.00108	0.00060	0.00031	0.00015
H2O	0.09779	0.10720	0.11469	0.12044	0.12472	0.12782	0.13001	0.13251	0.13356
NO	0.02470	0.02211	0.01946	0.01682	0.01428	0.01189	0.00970	0.00773	0.00533
NO2	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00000
N2	0.69173	0.70044	0.70725	0.71248	0.71647	0.71950	0.72180	0.72356	0.72590
O	0.02404	0.01641	0.01081	0.00685	0.00416	0.00241	0.00132	0.00069	0.00033
OH	0.03306	0.02711	0.02147	0.01645	0.01218	0.00871	0.00500	0.00397	0.00251
O2	0.109912	0.10447	0.10913	0.11311	0.11644	0.11919	0.12141	0.12319	0.12458
ADD H2O(L)									

CASE= 0		O/F=100.0000		F/A= 0.01000		PERCENT FUEL= 0.9901		PHI= 0.3430	
P, ATM	0.5000	0.5000	0.5000	0.5000	0.5000	0.5000	0.5000	0.5000	0.5000
P, PSIA	7.3	7.3	7.3	7.3	7.3	7.3	7.3	7.3	7.3
T, DEG K	1500.0	1400.0	1300.0	1200.0	1100.0	1000.0	900.0	800.0	700.0
T, DEG F	2240.3	2050.3	1880.3	1700.3	1520.3	1360.3	1160.3	980.3	800.3
RHO, G/CC	1.1087-4	1.1879-4	1.2793-4	1.3859-4	1.5119-4	1.6631-4	1.8479-4	2.0788-4	2.3728-4
M, MOL WT	27.292	27.293	27.293	27.293	27.293	27.293	27.293	27.293	27.293
CP, CAL/(G)(K)	0.3253	0.3197	0.3144	0.3091	0.3038	0.2982	0.2922	0.2857	0.2790
GAMMA(S)	1.2886	1.2950	1.3014	1.3081	1.3152	1.3230	1.3319	1.3421	1.3531
SON VEL,M/SEC	767.4	743.2	717.9	691.5	663.9	634.8	604.3	571.9	537.7
MOLE FRACTIONS									
AR	0.00870	0.00870	0.00870	0.00870	0.00870	0.00870	0.00870	0.00870	0.00870
CO	0.00028	0.00028	0.00028	0.00028	0.00028	0.00028	0.00028	0.00028	0.00028
CO2	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
H2O	0.13400	0.13403	0.13405	0.13405	0.13406	0.13406	0.13406	0.13406	0.13406
NO	0.00099	0.00059	0.00033	0.00016	0.00007	0.00003	0.00001	0.00000	0.00000
N2	0.72803	0.72825	0.72838	0.72847	0.72851	0.72854	0.72855	0.72855	0.72855
OH	0.00010	0.00004	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
O2	0.12789	0.12811	0.12825	0.12833	0.12838	0.12840	0.12841	0.12842	0.12842

TABLE II.—LISTING OF PARAMETER VARIATIONS FOR FIGURES 1 to 6

Figure	Fuel-air ratio (weight)	(Fuel-air ratio)/(stoichiometric fuel-air ratio), $\phi$	Initial temperature, K	Equilibrium temperature, K	Temperature rise, K, kelvins	Combustion pressure, atm	Mixture temperature, K	$\gamma(s)$	Molecular weight
1(a)	0.000-0.040	-----	250-1150	500-2600	-----	0.5-4.0	-----	-----	-----
(b)	.020-0.060	-----	↓	2600-2100	-----	0.5-4.0	-----	-----	-----
(c)	.000-0.040	-----	↓	500-2700	-----	4.0-50.0	-----	-----	-----
(d)	.020-0.060	-----	↓	2700-2100	-----	4.0-50.0	-----	-----	-----
2(a)	0.000-0.050	-----	250-1200	250-2635	-----	0.5	-----	-----	-----
(b)	↓	-----	↓	250-2685	-----	1.0	-----	-----	-----
(c)	↓	-----	↓	250-2710	-----	1.5	-----	-----	-----
(d)	↓	-----	↓	250-2730	-----	2.0	-----	-----	-----
(e)	↓	-----	↓	250-2750	-----	3.0	-----	-----	-----
(f)	↓	-----	↓	250-2770	-----	4.0	-----	-----	-----
(g)	↓	-----	↓	250-2790	-----	6.0	-----	-----	-----
(h)	↓	-----	↓	250-2825	-----	10.0	-----	-----	-----
(i)	↓	-----	↓	250-2840	-----	15.0	-----	-----	-----
(j)	↓	-----	↓	250-2850	-----	20.0	-----	-----	-----
(k)	↓	-----	↓	250-2870	-----	30.0	-----	-----	-----
(l)	↓	-----	↓	250-2885	-----	40.0	-----	-----	-----
(m)	↓	-----	↓	250-2895	-----	50.0	-----	-----	-----
3(a)	0.000-0.050	-----	250-1200	-----	0-2110	0.5	-----	-----	-----
(b)	↓	-----	↓	-----	0-2130	1.0	-----	-----	-----
(c)	↓	-----	↓	-----	0-2140	1.5	-----	-----	-----
(d)	↓	-----	↓	-----	0-2150	2.0	-----	-----	-----
(e)	↓	-----	↓	-----	0-2160	3.0	-----	-----	-----
(f)	↓	-----	↓	-----	0-2165	4.0	-----	-----	-----
(g)	↓	-----	↓	-----	0-2175	6.0	-----	-----	-----
(h)	↓	-----	↓	-----	0-2180	10.0	-----	-----	-----
(i)	↓	-----	↓	-----	0-2190	15.0	-----	-----	-----
(j)	↓	-----	↓	-----	0-2195	20.0	-----	-----	-----
(k)	↓	-----	↓	-----	0-2200	30.0	-----	-----	-----
(l)	↓	-----	↓	-----	0-2205	40.0	-----	-----	-----
(m)	↓	-----	↓	-----	0-2210	50.0	-----	-----	-----
4(a)	0.000-0.02916	-----	-----	-----	-----	0.5	300-2800	1.400-1.130	-----
(b)	↓	-----	-----	-----	-----	1.0	↓	1.400-1.137	-----
(c)	↓	-----	-----	-----	-----	1.5	↓	1.400-1.143	-----
(d)	↓	-----	-----	-----	-----	2.0	↓	1.400-1.146	-----
(e)	↓	-----	-----	-----	-----	3.0	↓	1.400-1.152	-----
(f)	↓	-----	-----	-----	-----	4.0	↓	1.400-1.156	-----
(g)	↓	-----	-----	-----	-----	6.0	↓	1.400-1.161	-----
(h)	↓	-----	-----	-----	-----	10.0	↓	1.400-1.168	-----
(i)	↓	-----	-----	-----	-----	15.0	↓	1.400-1.174	-----
(j)	↓	-----	-----	-----	-----	20.0	↓	1.400-1.177	-----
(k)	↓	-----	-----	-----	-----	30.0	↓	1.400-1.182	-----
(l)	↓	-----	-----	-----	-----	40.0	↓	1.400-1.186	-----
(m)	↓	-----	-----	-----	-----	50.0	↓	1.400-1.188	-----
5(a)	0.000-0.02916	-----	-----	-----	-----	0.5	300-2800	-----	28.97-23.10
(b)	↓	-----	-----	-----	-----	1.0	↓	-----	28.97-23.48
(c)	↓	-----	-----	-----	-----	1.5	↓	-----	28.97-23.64
(d)	↓	-----	-----	-----	-----	2.0	↓	-----	28.97-23.75
(e)	↓	-----	-----	-----	-----	3.0	↓	-----	28.97-23.87
(f)	↓	-----	-----	-----	-----	4.0	↓	-----	28.97-23.95
(g)	↓	-----	-----	-----	-----	6.0	↓	-----	28.97-24.05
(h)	↓	-----	-----	-----	-----	10.0	↓	-----	28.97-24.15
(i)	↓	-----	-----	-----	-----	15.0	↓	-----	28.97-24.21
(j)	↓	-----	-----	-----	-----	20.0	↓	-----	28.97-24.25
(k)	↓	-----	-----	-----	-----	30.0	↓	-----	28.97-24.30
(l)	↓	-----	-----	-----	-----	40.0	↓	-----	28.97-24.34
(m)	↓	-----	-----	-----	-----	50.0	↓	-----	28.97-24.36
6(a)	-----	0.10-1.00	250-1250	585-2635	-----	0.5	-----	-----	-----
(b)	-----	↓	↓	585-2680	-----	1.0	-----	-----	-----
(c)	-----	↓	↓	585-2710	-----	1.5	-----	-----	-----
(d)	-----	↓	↓	585-2725	-----	2.0	-----	-----	-----
(e)	-----	↓	↓	585-2755	-----	3.0	-----	-----	-----
(f)	-----	↓	↓	585-2770	-----	4.0	-----	-----	-----
(g)	-----	↓	↓	585-2795	-----	6.0	-----	-----	-----
(h)	-----	↓	↓	585-2825	-----	10.0	-----	-----	-----
(i)	-----	↓	↓	585-2845	-----	15.0	-----	-----	-----
(j)	-----	↓	↓	585-2860	-----	20.0	-----	-----	-----
(k)	-----	↓	↓	585-2880	-----	30.0	-----	-----	-----
(l)	-----	↓	↓	585-2890	-----	40.0	-----	-----	-----
(m)	-----	↓	↓	585-2900	-----	50.0	-----	-----	-----

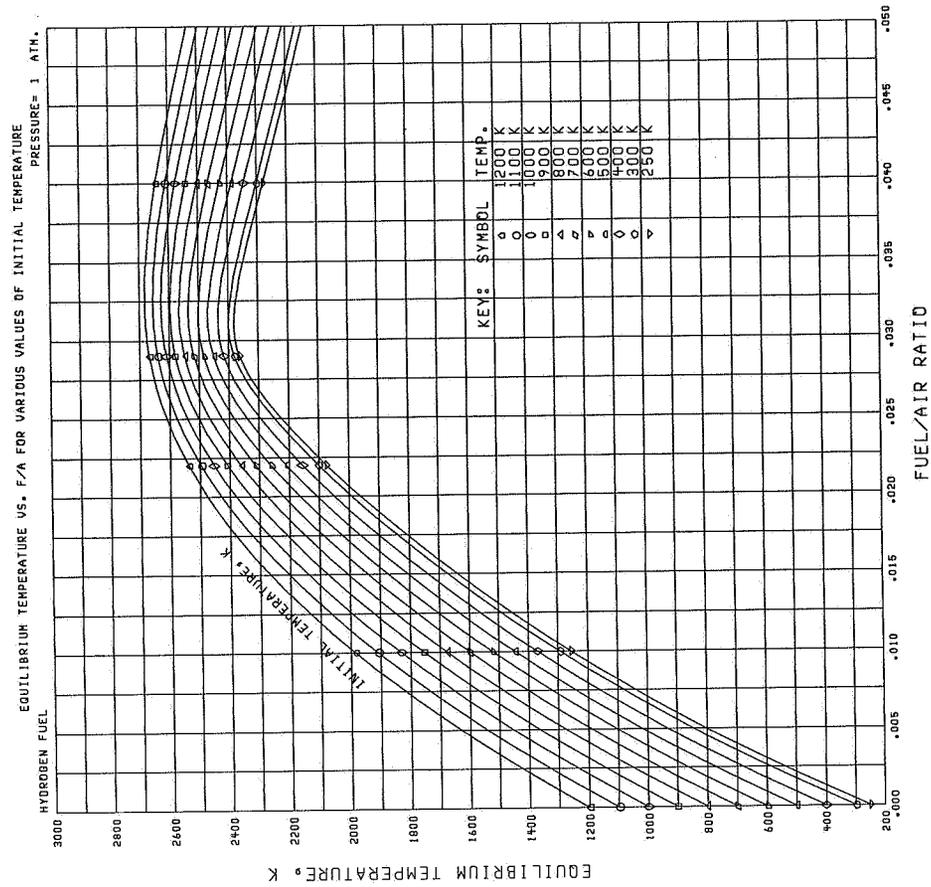


Figure 2.—Equilibrium temperature as function of initial temperature and fuel-air ratio at pressure of 1 atmosphere. Reproduction of microfiche figure 2(b).

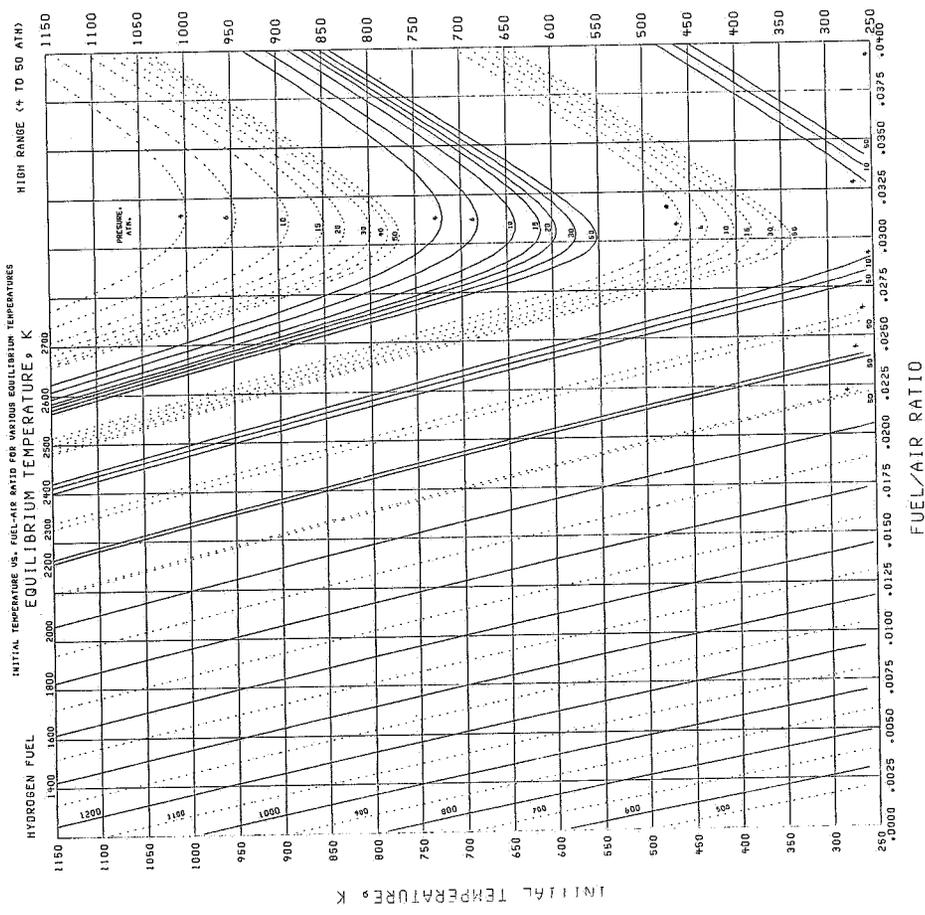


Figure 1.—Equilibrium temperature as function of initial temperature, fuel-air ratio, and pressure range of 4 to 50 atmospheres. Reproduction of microfiche figure 1(c).

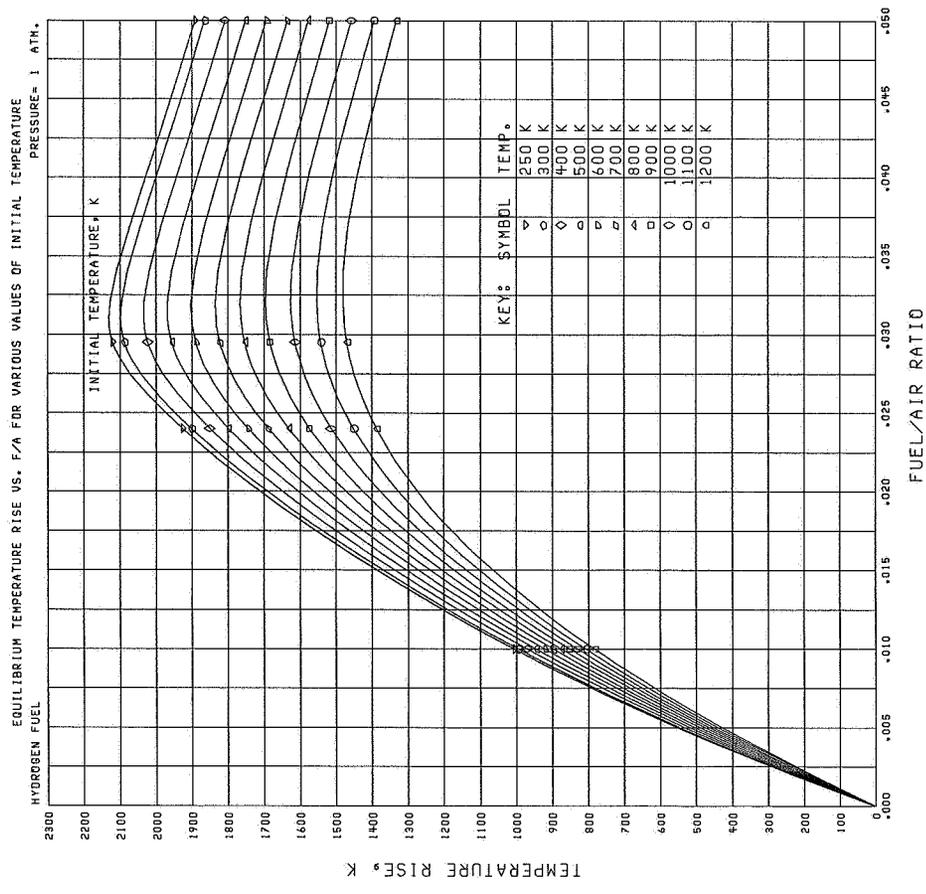


Figure 3.—Equilibrium temperature rise as function of initial temperature and fuel-air ratio at pressure of 1 atmosphere. Reproduction of microfiche figure 3(b).

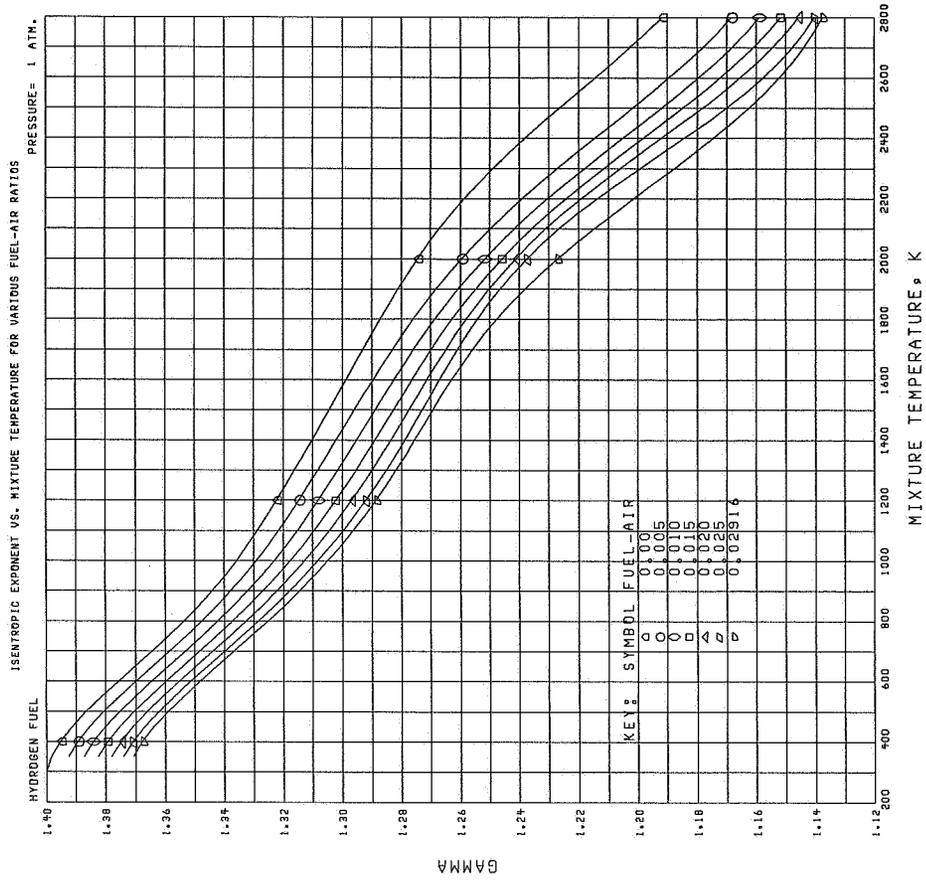


Figure 4.— $\gamma(s)$  as function of mixture temperature and fuel-air ratio at pressure of 1 atmosphere. Reproduction of microfiche figure 4(b).

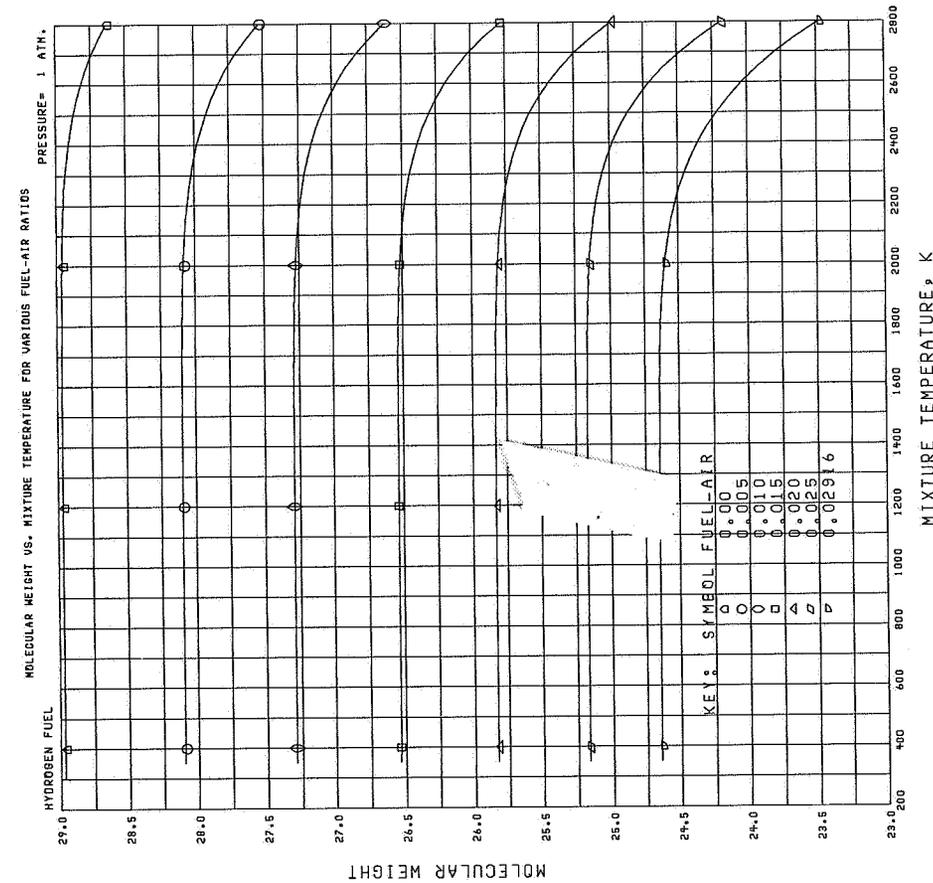


Figure 5.—Molecular weight as function of mixture temperature and fuel-air ratio at pressure of 1 atmosphere. Reproduction of microfiche figure 5(b).

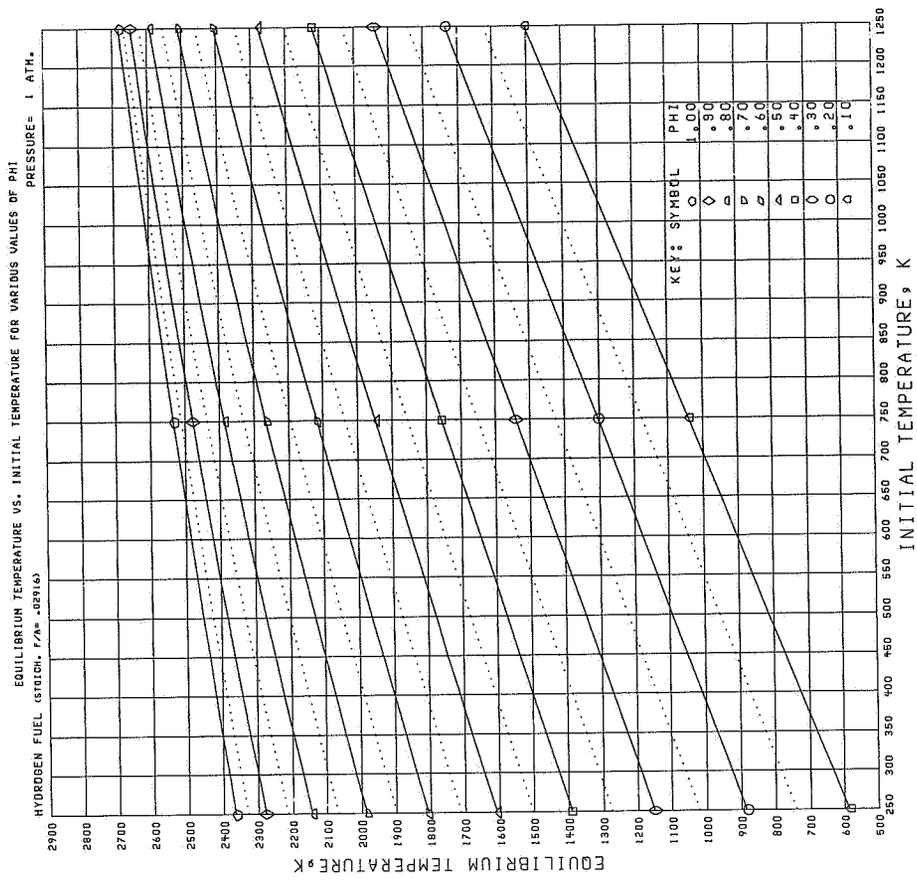


Figure 6.—Equilibrium temperature as function of initial temperature and equivalence ratio  $\phi$  at pressure of 1 atmosphere. Reproduction of microfiche figure 6(b).

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16. Abstract A series of computations has been made to produce the equilibrium temperature and gas composition for hydrogen gas fuel and dry air. The computed tables and figures provide combustion gas property data for pressures from 0.5 to 50 atmospheres and equivalence ratios from 0 to 2.0. Only sample tables and figures are provided in this report. The complete set of tables and figures is provided on four microfiche films supplied with this report.					
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