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Combustion Gas Properties of Various Fuels of Interest to Gas Turbine Engineers

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ABSTRACT

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A series of computations have been made using the gas property computational schemes of Gordon and McBride to compute the gas properties and species concentration of ASTM-Jet A and dry air. The purpose of this work was to present the computed gas thermodynamic properties in a revised graphical format that would present this information in a way very useful to combustion engineers. The plan is to publish an extensive series of reports covering the properties of many fuel and air combinations. The revised graphical presentation displays on one chart the output from hundreds of computer sheets. The published reports will contain microfiche cards, from which complete tables and graphs can be obtained. This report documents the extent of the planned effort and provides samples of the many tables and charts that will be available on the microfiche cards.

INTRODUCTION

The purpose of this paper is twofold: it is first to acquaint the reader with the present activity at NASA Lewis where combustion gas properties of many fuel and air combinations are being computed and second to elicit additional input from the technical combustion community as to additional fuel-air combinations that should be computed.

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 extensively used both at NASA and throughout the industry. The computational schemes that have been developed over the years by Huff, Gordon, Morrell, 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, as for instance Ref. 5. This work can be used to obtain the desired values of gas property for specific fuels, but requires that multiple extrapolations be made to account for the proper value of fuel carbon-to-hydrogen ratio, inlet-air temperature, fuel-air ratio, and pressure. In addition to being tedious to use, tables fail to graphically portray the influence, or lack of influence, of the various parameters on a combustion gas property.

The information on combustion gas properties obtainable from the referenced works has been put together in an entirely different format as a series of tables and charts. These charts have proven to be extremely useful in combustion research and copies of such charts have been prepared in the past for a wide variety of fuels. Due to the numerous requests for these charts as well as the interest in high pressure combustion research, Ref. 9, we have decided to prepare a new series of charts and tables and extend the applicable range of parameters covered.

This paper will present sample tables and thermodynamic charts of the type that will be included in each report. At the present time, reports covering the gas properties of ASTM-Jet A and dry air, and

natural gas and dry air, are being published. Combustion gas properties have been computed for a range of pressures from 0.5 to 50 atm, inlet-air temperatures from 250 to 1150 K and equivalence ratios from 0 to 2. The complete tables and figures will not be reproduced in each report; only sample figures are provided. The complete tables and charts are provided on microfiche cards supplied with each report.

SCOPE

The complete preparation and publication of these combustion gas property charts is expected to take several years. This is particularly true if the number of planned fuel-oxidant combinations should increase. Table I is a listing of the fuel and oxidant combinations that are planned for computation. Additions or deletions can be made in response to the interest we receive for this work. The computational scheme that has been devised, using the programs developed in Refs. 4, 6 to 8 permits one to generate these tables and charts of gas properties with relative ease.

PROCEDURE

The computations of combustion gas properties are performed using the computer routines that have been developed by Gordon, McBride et al. and are documented in detail in Refs. 5 to 8. The computational codes have been extensively utilized in the past to generate tables of combustion gas properties. The most recent publication of tables is to be found in Ref. 5. In this referenced work, combustion gas properties were computed for parametric values of hydrogen to carbon ratios, rather than specific ratios representative of actual fuels. The graphs and tables shown in the present report were made specifically for the fuel-oxidant choice of ASTM-Jet A and dry air. An average molecular carbon-to-hydrogen ratio of 1.9067 was used for the computation. This value was an average obtained from analysis of several samples of ASTM-Jet A, a wide specification range kerosene-type, commercial grade aviation fuel. Calculation of combustion gas properties was performed using the referenced computer codes. Normally, many hundreds of pages of computer printouts would be obtained in order to amass the information required to generate the appropriate graphs. The computer program has been modified slightly to avoid the problems of cross-plotting this information by hand and can now directly generate the tables and charts useful to combustion engineers. For example, charts of equilibrium gas temperature were generated over a range of inlet-air temperatures, pressures, and fuel-air ratios. This has been done by selecting a constant value for the equilibrium temperature, a pressure and fuel-air ratio, and then computing in an iterative manner the required value of the inlet-air temperature. Computed values are stored as a data set and charts are produced by the computer. In regions where the results become highly nonlinear, additional computations are performed to present the results with the desired level of accuracy. A careful examination of the charts in these regions will show

that the curve fit consists of very short linear segments. Nonetheless, the appropriate level of accuracy that one needs from such charts is still provided.

In a similar fashion, an appropriate iterative procedure was used to generate the other gas property charts.

RESULTS

The computation procedure was used to generate the tables and charts that will be presented in each subsequent report. The bulk of the information that was generated is presented on microfiche cards provided with each report. Sample tables and figures are presented in this paper to illustrate the nature of the information that is available.

Tabular Listings

Table II of this report is a copy of a typical listing of combustion gas properties and species. Included in these tables are the following:

1. Case number and description which includes the oxidant-fuel ratio (O/F), the fuel-air ratio, (F/A), percent fuel, and the equivalence ratio (Φ). The change in case number has been used to specify a change in the inlet-air temperature; e.g., case 1 is 250 K, in Case 2 is 400 K (shown), case 7 is 1150 K.

2. Combustion gas properties which are equilibrium temperature (K), density (g/cc), molecular weight, specific heat at constant pressure, (cal/g-K), isentropic exponent- γ (s), and sonic velocity (m/sec).

3. Mole fractions of the various gas species are given when their concentration is equal to or greater than 5 ppmv.

The listing at the top of Table II is the input information on the fuel and oxidant. Listed are, reading from left to right, the fuel and oxidant atomic formulas, the weight fraction of each component, the heats of formation, the inlet temperature (fuel was always introduced at 298 K and air for Case 2 is at 400 K), and the density of the fuel in the last column. This is typical input listing that is used by Gordon in Ref. 5.

The tables list the gas properties and species concentrations for 1820 different combinations of parametric conditions. The parameters and values used are listed below.

Combustion pressure, atm.: 0.5, 1, 1.5, 2, 3, 4, 6, 10, 15, 20, 30, 40, 50

Inlet-air temperature, K: 250, 400, 600, 800, 1000, 1100, 1150 (cases 1 to 7.)

Equivalence ratio, Φ (Φ): 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

The information contained in these tables has been used to generate the thermodynamic properties shown in Figs. 1 to 3, and 6.

Table III presents a sample of another type of tabular listing supplied in these reports. These tables list thermodynamic combustion gas properties for different combinations of parametric conditions. These tables were computed by selecting the combustion pressure, mixture temperature, and fuel-air ratio and then performing iterative calculations to generate the properties of these combustion gas mixtures. The parameters used and ranges were:

Combustion pressure, atm: 0.5 to 50 (in steps as indicated above)

Mixture temperature, K: 2800 to 300 in 100 K increments

Fuel-air-ratio (weight): 0.0 to 0.1 in increments of 0.01

Information contained in these tables has been used to generate the thermodynamic properties shown in Fig. 4 and 5.

Graphical Presentations of Thermodynamic Properties

Some typical figures have been included in this paper to illustrate the nature of the charts that are available on the report microfiche cards. Figure 1 presents computed values showing the effect of varying the inlet-air temperature, the fuel-air ratio, and the combustion pressure on the equilibrium gas temperature. The figure covers a range of pressures from 4 to 50 atmospheres. Curves at lower pressures (0.5 to 4 atm.) are available on the microfiche cards, but were not included on this figure as the curves tend to overlap and become confusing.

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

Figure 3 is similar to Fig. 2 except that temperature rise values are plotted versus the fuel-air ratio for a range of inlet-air temperatures at the 1 atm pressure level. Curves at other pressure levels are available on the microfiche cards. Figure 4 presents the variation in the isentropic exponent, γ (s), as a function of the gas mixture temperature for various values of fuel-air ratio at a single value of combustion pressure; again 1 atmosphere for the illustrated figure. For the purpose of these reports, 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 values of fuel-air ratio at specified levels of combustion pressure.

Figure 6 shows the relationship between the computed equilibrium temperature for various values of the equivalence ratio, Φ (Φ), at specified pressure levels.

SUMMARY

The computational schemes that have been used in the past to compute thermodynamic combustion gas properties have been modified to generate a series of tables and charts that are believed to be particularly useful for gas turbine combustion engineers. At present, reports covering the thermodynamic properties and species concentration of ASTM-Jet A and dry air, and natural gas and dry air, are complete and in publication.

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TABLE I. - LIST OF PLANNED FUEL-OXIDANT COMBINATIONS

- | | |
|-------------------------------|---------------------------------|
| 1. Jet-A and Air | 15. Propane and Air |
| 2. Jet-A and Air + 2% Oxygen | 16. ERBS + 2% Methanol and Air |
| 3. Jet-A and Air + 4% Oxygen | 17. ERBS + 4% Methanol and Air |
| 4. JET-A and Air + 6% Oxygen | 18. ERBS + 6% Methanol and Air |
| 5. JET-A and Air + 8% Oxygen | 19. ERBS + 8% Methanol and Air |
| 6. JET-A and Air + 10% Oxygen | 20. ERBS + 10% Methanol and Air |
| 7. JET-A and Humid Air | 21. Low BTU Gas and Air |
| 8. JP-4 and Air | 22. Medium BTU Gas and Air |
| 9. ERBS and Air | 23. Hydrogen and Air |
| 10. Gasoline and Air | 24. JP-10 and Air |
| 11. Natural Gas and Air | 25. JP-10 + 50% Carbon and Air |
| 12. Methane and Air | 26. JP-10 + Aluminum and Air |
| 13. Methane @ 589K and Air | 27. JP-10 + Boron and Air |
| 14. Methane @ 922K and Air | |

TABLE II. - EXAMPLE OF MICROFICHE TABULAR LISTING OF COMPUTED GAS PROPERTIES: EQUILIBRIUM TEMPERATURE DETERMINATION

[illegible]

TABLE III. - EXAMPLE OF MICROFICHE TABULAR LISTING OF COMPUTED GAS PROPERTIES: AT
SELECTED MIXTURE TEMPERATURES

| CASE= 0 | | O/F=100.0000 | | F/A= 0.01000 | | PERCENT FUEL= | | 0.9901 | | PHI= 0.1665 | |
|----------------|----------|--------------|----------|--------------|----------|---------------|----------|----------|----------|-------------|----------|
| P, ATM | 0 | 0.5000 | 0.5000 | 0.5000 | 0.5000 | 0.5000 | 0.5000 | 0.5000 | 0.5000 | 0.5000 | 0.5000 |
| T, DEG K | 1500.0 | 1400.0 | 1300.0 | 1200.0 | 1100.0 | 1000.0 | 900.0 | 800.0 | 700.0 | 600.0 | 500.0 |
| T, DEG F | 2200.0 | 2060.0 | 1880.0 | 1700.0 | 1520.0 | 1340.0 | 1160.0 | 980.0 | 800.0 | 620.0 | 440.0 |
| RHO, G/CC | 1.1767-4 | 1.2607-4 | 1.3577-4 | 1.4709-4 | 1.6046-4 | 1.7651-4 | 1.9612-4 | 2.2083-4 | 2.5213-4 | 2.9418-4 | 3.5010-4 |
| M, MOL/WT | 28.967 | 28.967 | 28.967 | 28.967 | 28.967 | 28.967 | 28.967 | 28.967 | 28.967 | 28.967 | 28.967 |
| CP, CAL/(G)(K) | 0.2996 | 0.2950 | 0.2864 | 0.2774 | 0.2680 | 0.2586 | 0.2492 | 0.2400 | 0.2308 | 0.2216 | 0.2124 |
| GAMMA (S) | 1.2971 | 1.3050 | 1.3089 | 1.3151 | 1.3215 | 1.3285 | 1.3369 | 1.3466 | 1.3574 | 1.3688 | 1.3803 |
| SON VEL, M/SEC | 747.3 | 723.6 | 698.9 | 673.0 | 645.9 | 617.5 | 587.7 | 556.1 | 522.2 | 485.5 | 445.0 |
| MOLE FRACTIONS | | 0.00923 | | 0.00923 | | 0.00923 | | 0.00923 | | 0.00923 | |
| AR | 0.00923 | 0.00923 | 0.00923 | 0.00923 | 0.00923 | 0.00923 | 0.00923 | 0.00923 | 0.00923 | 0.00923 | 0.00923 |
| CO2 | 0.02088 | 0.02088 | 0.02088 | 0.02088 | 0.02088 | 0.02088 | 0.02088 | 0.02088 | 0.02088 | 0.02088 | 0.02088 |
| H2O | 0.01960 | 0.01962 | 0.01962 | 0.01962 | 0.01962 | 0.01962 | 0.01962 | 0.01962 | 0.01962 | 0.01962 | 0.01962 |
| N2 | 0.00120 | 0.00072 | 0.00039 | 0.00020 | 0.00009 | 0.00003 | 0.00001 | 0.00000 | 0.00000 | 0.00000 | 0.00000 |
| OH | 0.77262 | 0.77287 | 0.77303 | 0.77313 | 0.77319 | 0.77321 | 0.77322 | 0.77323 | 0.77323 | 0.77323 | 0.77323 |
| O2 | 0.00042 | 0.00002 | 0.00001 | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 |
| CASE= 0 | | O/F=100.0000 | | F/A= 0.01000 | | PERCENT FUEL= | | 0.9901 | | PHI= 0.1665 | |
| P, ATM | 0 | 0.5000 | 0.5000 | 0.5000 | 0.5000 | 0.5000 | 0.5000 | 0.5000 | 0.5000 | 0.5000 | 0.5000 |
| T, DEG K | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| T, DEG F | 2800.0 | 2700.0 | 2600.0 | 2500.0 | 2400.0 | 2300.0 | 2200.0 | 2100.0 | 2000.0 | 1900.0 | 1800.0 |
| RHO, G/CC | 4580.3 | 4400.3 | 4220.3 | 4040.3 | 3860.3 | 3680.3 | 3500.3 | 3320.3 | 3140.3 | 2960.3 | 2780.3 |
| M, MOL/WT | 1.2382-4 | 1.2911-4 | 1.3462-4 | 1.4042-4 | 1.4657-4 | 1.5315-4 | 1.6026-4 | 1.6788-4 | 1.7644-4 | 1.8561-4 | 1.9566-4 |
| CP, CAL/(G)(K) | 0.6154 | 0.5303 | 0.4936 | 0.4667 | 0.4494 | 0.4308 | 0.4193 | 0.4053 | 0.3894 | 0.3725 | 0.3554 |
| GAMMA (S) | 1.1745 | 1.1836 | 1.1947 | 1.2072 | 1.2202 | 1.2339 | 1.2486 | 1.2641 | 1.2801 | 1.2964 | 1.3129 |
| SON VEL, M/SEC | 980.4 | 963.8 | 948.3 | 933.3 | 918.4 | 903.1 | 887.1 | 870.1 | 852.0 | 833.0 | 812.9 |
| MOLE FRACTIONS | | 0.00923 | | 0.00923 | | 0.00923 | | 0.00923 | | 0.00923 | |
| AR | 0.00907 | 0.00912 | 0.00915 | 0.00918 | 0.00920 | 0.00921 | 0.00922 | 0.00922 | 0.00923 | 0.00923 | 0.00923 |
| CO | 0.00574 | 0.00608 | 0.00623 | 0.00635 | 0.00645 | 0.00653 | 0.00660 | 0.00666 | 0.00671 | 0.00676 | 0.00681 |
| H2O | 0.01477 | 0.01454 | 0.01428 | 0.01400 | 0.01371 | 0.01341 | 0.01310 | 0.01278 | 0.01245 | 0.01211 | 0.01177 |
| N2 | 0.00013 | 0.00010 | 0.00007 | 0.00004 | 0.00002 | 0.00001 | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 |
| OH | 0.00069 | 0.00051 | 0.00036 | 0.00024 | 0.00015 | 0.00009 | 0.00005 | 0.00003 | 0.00001 | 0.00000 | 0.00000 |
| O2 | 0.01210 | 0.01173 | 0.01133 | 0.01094 | 0.01055 | 0.01015 | 0.00974 | 0.00932 | 0.00889 | 0.00846 | 0.00803 |
| N2O | 0.00002 | 0.00002 | 0.00002 | 0.00002 | 0.00002 | 0.00002 | 0.00002 | 0.00002 | 0.00002 | 0.00002 | 0.00002 |
| N2 | 0.74588 | 0.74963 | 0.75344 | 0.75722 | 0.76100 | 0.76479 | 0.76855 | 0.77229 | 0.77601 | 0.77971 | 0.78339 |
| O | 0.02082 | 0.01410 | 0.00922 | 0.00580 | 0.00351 | 0.00202 | 0.00111 | 0.00057 | 0.00028 | 0.00012 | 0.00008 |
| OH | 0.00085 | 0.00099 | 0.00070 | 0.00057 | 0.00046 | 0.00035 | 0.00027 | 0.00020 | 0.00016 | 0.00012 | 0.00008 |
| O2 | 0.14877 | 0.15421 | 0.15871 | 0.16241 | 0.16546 | 0.16795 | 0.16999 | 0.17165 | 0.17299 | 0.17406 | 0.17466 |

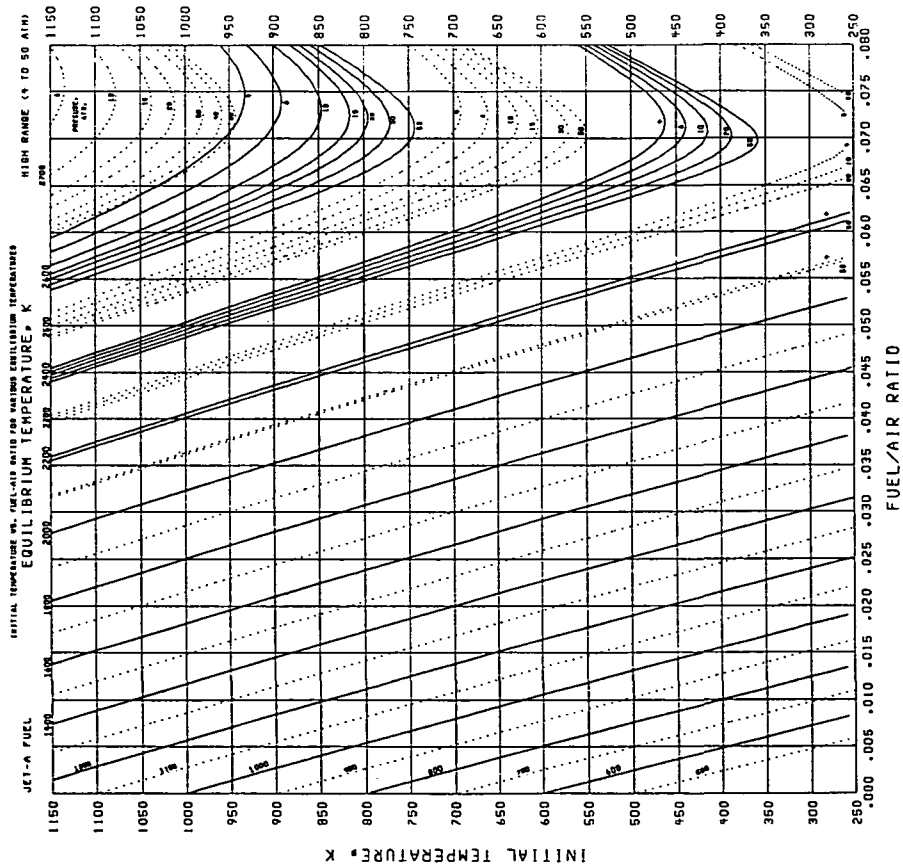


Figure 1. - Reproduction of microfiche figure 1(c): Equilibrium temperature as a function of initial temperature, fuel-air ratio, and a pressure range of 4 to 50 atmospheres.

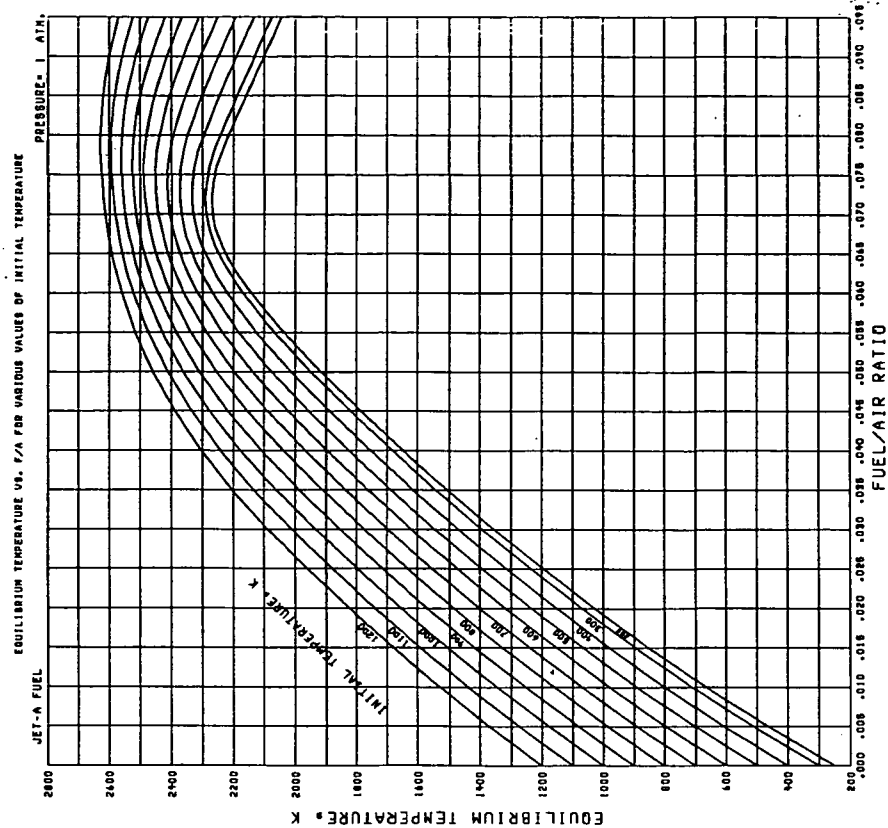


Figure 2. - Reproduction of microfiche figure 2(b): Equilibrium temperature as a function of initial temperature and fuel-air ratio at a pressure of 1 atmosphere.

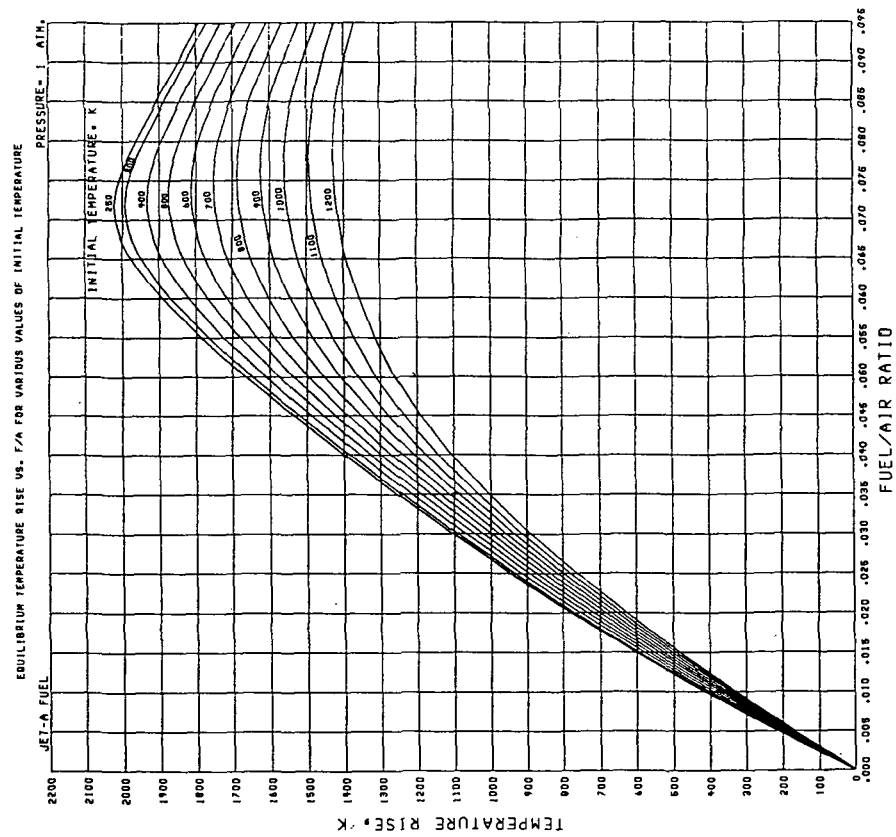


Figure 3. - Reproduction of microfiche figure 3(b): Equilibrium temperature rise as a function of initial temperature and fuel-air ratio at a pressure value of 1 atmosphere.

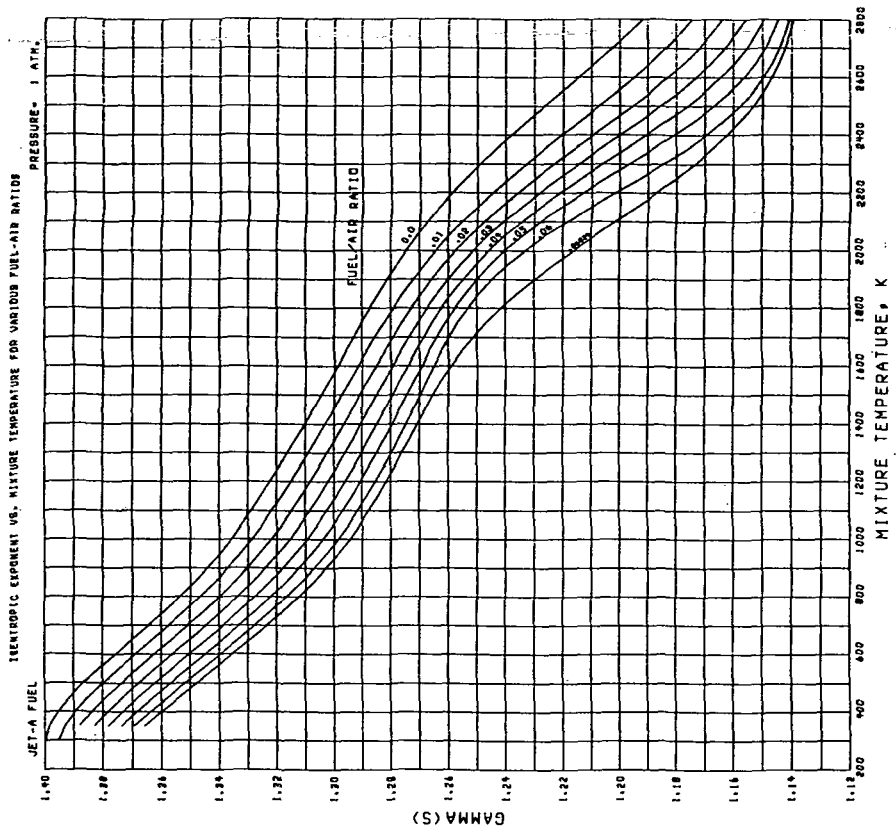


Figure 4. - Reproduction of microfiche figure 4(b): Gamma(s) as a function of mixture temperature and fuel-air ratio at 1 atmosphere pressure.

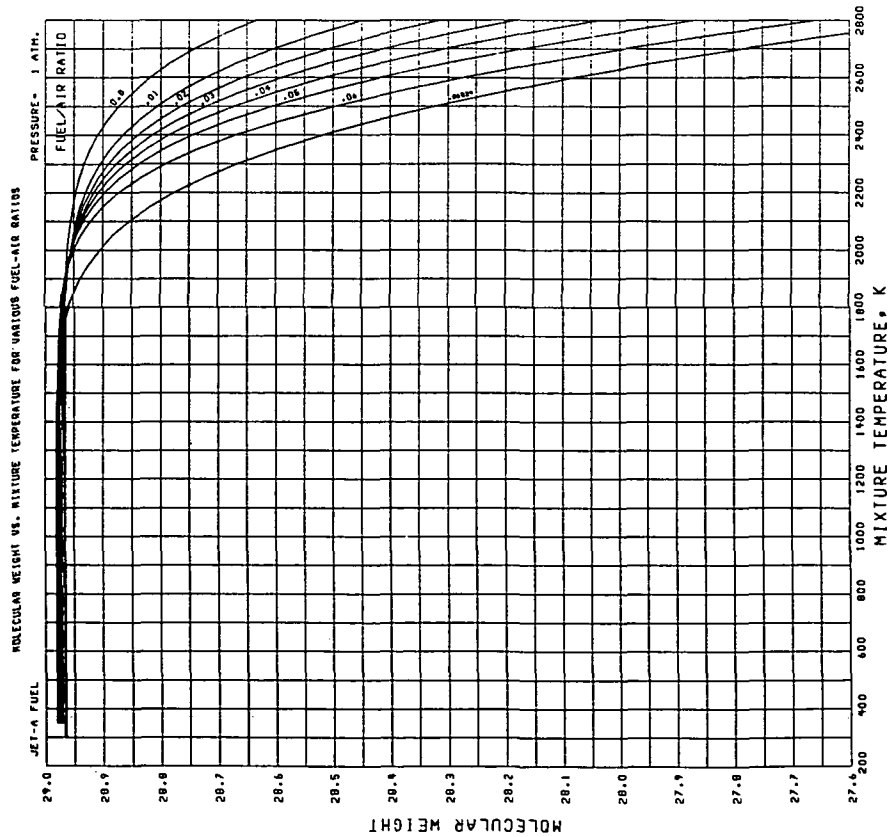


Figure 5. - Reproduction of microfiche figure 5(b): Molecular weight as a function of mixture temperature and fuel-air ratio at a pressure of 1 atmosphere.

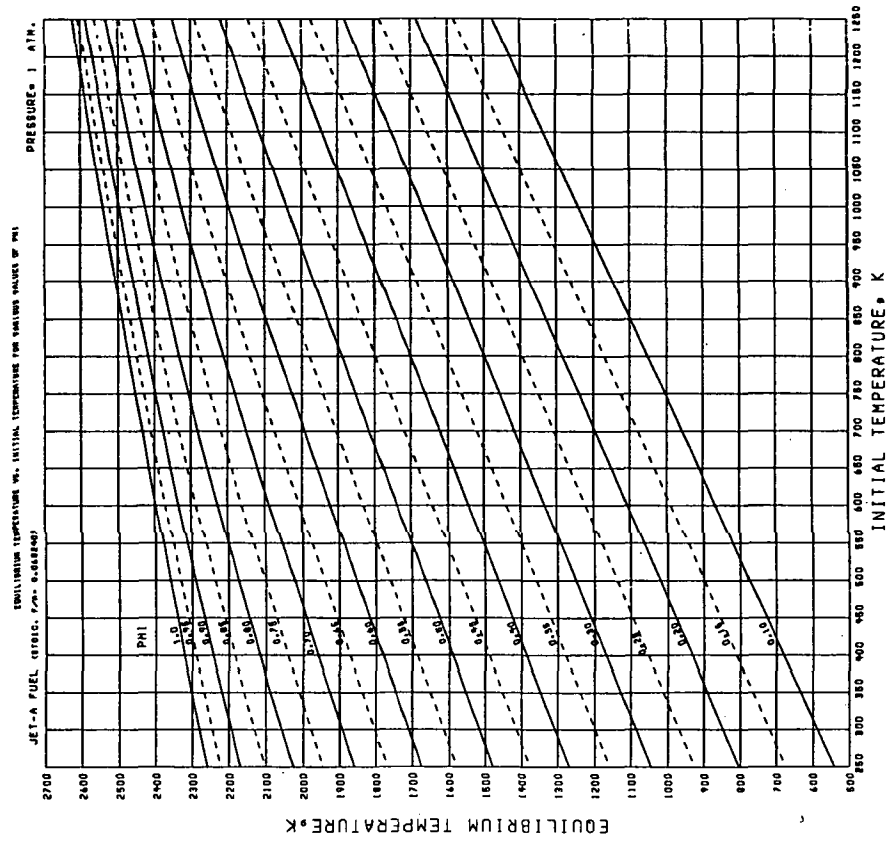


Figure 6. - Reproduction of microfiche figure 6(b): Equilibrium temperature as a function of initial temperature and equivalence ratio phi at 1 atmosphere pressure.

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